Telemac-Mascaret System

Developer Guide

Version v8p2

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Contents

1. Foreword

This is the lastest release of the developer guide to the TELEMAC-MASCARET SYSTEM, based on FORTRAN 2003. It has been written to help the numerous people who have to develop or to understand the "ins" and "outs" of this system, namely research engineers and technicians at EDF, students and researchers in universities, research institutes and laboratories, or users willing to write specific user subroutines. It will probably not meet all the expectations: giving fully detailed explanations on all the system would take thousands of pages, and would probably never be read! With this guide we only hope to establish a closer relationship between developers, and we shall enhance the guide progressively, as new questions arise. This document will be a success if you consider it yours. We thus beg you to report on errors, misprints and mistakes, and to ask for more explanations on parts that would not be clear enough. It will be a commitment for us to take into account all your remarks in next releases.

2. Structure of this guide

This guide is made of four main parts and a number of appendices. Chapter 4 should be the only useful one for developers of programs based on the BIEF library. Chapter 5 give details on the very structure of BIEF and is *a priori* meant for BIEF developers themselves. Chapter 7 is about the different program a developer will have to use. Chapter 8 is the coding convention that should be followed when developping in TELEMAC-MASCARET SYSTEM.

3. Introduction

3.1 Why a finite element library?

A great many finite element software programs have been developed over the last few years at the Laboratoire National d'Hydraulique et Environnement. These have been based on a single data structure, initiated by the development of TELEMAC-2D. Algorithms used by one program, for example to process a diffusion operator, can also be used by another. It was therefore felt to be quite natural to group together all the numerical developments of the various codes in a single library, distinguishing them from the physical aspects.
This finite element library (called BIEF in the rest of this document. BIEF stands for the French expression **BI**bliothèque d'**E**lements **F**inis, meaning Finite Element Library, but "bief" in French is a river reach in English) is designed so that it can be used as a toolbox in the simplest possible way. It is possible, for example, to solve a classic fluid mechanics equation by calling the BIEF *ad hoc* modules, without having to worry about the details of the solution. This simplifies and considerably speeds up the calculation code development phase. In addition, BIEF continually includes new developments, thereby making them available to users immediately.
The development of BIEF is closely linked to that of the TELEMAC system codes, most of which are the subject of a Quality Control procedure. In the case of the software programs of the EDF's Research and Development, this procedure involves designing and then checking the quality of the product throughout the different phases in its life. In particular, a software program subjected to Quality Control is accompanied by a validation document which describes a series of test cases. This document can be used to evaluate the qualities and limitations of the product and identify its field of application. These test cases are also used for developing the software and are checked each time a modification is made. Consequently, the BIEF algorithms also benefit from this strict quality control procedure.

3.2 Brief description of BIEF

The data structure and programming of BIEF is described in detail in Part B of this document. One of the important features of this structure is that matrices are stored either in elementary form or in an edge-by-edge storage. Compared with compact storage, this type of storage saves on memory space for numerous types of elements and also enables resolution algorithms to be obtained quickly and efficiently. In fact, one of the essential features of BIEF is to offer methods with very low computing costs.

BIEF offers a whole range of subroutines. They include methods for solving advection equations, diffusion equations, linear system inversion methods with different types of preconditioning. The user is also provided with subroutines for calculating matrices: mass matrices, diffusion matrices, boundary matrices, etc. BIEF can be used to carry out all the conventional operations on vectors (norms, dot products, etc.), on the products of one matrix by a vector or of two matrices. By simply calling a subroutine, the user can calculate the divergence of a vector, the gradient of a function, and so on. It should be remembered that this description is not exhaustive and that the content of BIEF will change depending on the requirements of its users.
The language used is FORTRAN 90 (see explanations below), and, to facilitate the diffusion of the TELEMAC system, portability is checked on a wide range of hardware, including both super-computers and workstations, Linux and Windows machines.

3.3 Fortran 90: reasons for the change

TELEMAC was written in FORTRAN 77 up to version 3.2. There are a number of reasons for the choice of FORTRAN 90 for BIEF:

- Structured programming. Structures were prepared in version 3.2 of BIEF in FORTRAN 77, at the price of non-standard features, for example the use of negative indices in arrays. The structures are now normal structures in FORTRAN 90, and they are much easier to use.
- Dynamic allocation of memory.
- The increasing number of modules based on BIEF meant that it was taking longer and longer to complete each update. One of the aim of structured programming is to simplify updating.
- The increasing number of arguments in the subroutines, and changes of arguments in the user subroutines. This will is suppressed as far as possible by the use of FORTRAN 90 modules.

The principal objectives of structured programming are therefore:

- To enable dynamic allocation of memory.
- To facilitate update and development of the system elements.
- To facilitate the future development and maintenance of BIEF.
- To get a safer implementation, with many error checking done by the compiler itself.
- To enable a better compatibility between subsequent versions of BIEF.

4. Programming with BIEF

4.1 Features of Fortran 90 used in BIEF:

We briefly explain hereafter features of FORTRAN 90 that are used in BIEF. For more detailed explanations please refer to a real Fortran 90 book, such as M. and J. [7].

4.1.1 Structures

FORTRAN 77 only recognises integers, real numbers, Boolean and character strings. FORTRAN 90 can be used to create structures. The following is an example of the creation of a 'point' type structure composed of two real numbers, and a circle structure, composed of a centre and a radius:

```
TYPE point
  REAL :: x,y
END TYPE
!
TYPE circle
  TYPE(point) :: centre
  REAL :: radius
END TYPE
```

It can be observed that the centre is itself a structure of a type previously defined. Once the structure has been defined, objects of this type can be declared:

```
TYPE(circle) :: ROND
```

ROND will be a circle with its centre and radius; the latter are obtained thanks to the % "component selector". Thus the radius of `ROND` will be the real `ROND%radius`.

4.1.2 Pointers

Pointers are well known in C language, but are notably different in Fortran 90. Pointers in Fortran 90 may be used as pointers as in C but also as aliases. Unlike C, they are not mere addresses pointing to somewhere in the computer memory. The target must be defined precisely, for example the line:

```
REAL, POINTER, DIMENSION(:) :: X
```

will define a pointer to a one-dimensional real array, and it will be impossible to have it pointing to an integer nor even to a 2-dimensional array. This pointer X will have then to be pointed to a target by the statement:

```
X => Y
```

where Y is an already existing one-dimensional real array. Then X can be used as if it were Y, it is thus an alias.
X can be also directly allocated as a normal array by the statement:

```
ALLOCATE(X(100))
```

to have (for example) an array of 100 values. In this case X and its target have the same name. A well known problem in Fortran 90 is the fact that arrays of pointers do not exist. To overcome this problem, one has to create a new structure which is itself a pointer, and to declare an array of this new structure. This is done for blocks, which are lists of pointers to `BIEF_OBJ` structures.

4.1.3 Modules

Modules are like INCLUDE statements, but are more clever, so that INCLUDE should now always be avoided. As a matter of fact, modules can be used to define global variables that will be accessible to all routines. With the following module:

```
MODULE EXAMPLE
  INTEGER EX1,EX2,EX3,EX4
END MODULE EXAMPLE
```

all the subroutines beginning with the statement: `USE EXAMPLE` will have access to the same numbers `EX1,...EX4`. With `INCLUDE` statements, it would be only local variables without link to `EX1,...` declared in other subroutines.
Modules will thus be used to define global variables that will be accessed via a USE statement. If only one or several objects must be accessed, the ONLY statement may be used, as in the example below:

```
USE EXAMPLE, ONLY : EX1,EX2
```

This will enable to avoid name conflicts and secures programming.
Modules are also used to store interfaces that will be shared between several subroutines (see paragraph below)

4.1.4 Interfaces

Interfaces are a mean given to the compiler to check arguments of subroutines even if it has no access to them. For example, the following interface:

```
INTERFACE
  LOGICAL FUNCTION EOF(LUNIT)
    INTEGER, INTENT(IN) :: LUNIT
  END FUNCTION
END INTERFACE
```

says that function `EOF` has one integer argument. `INTENT(IN)` indicates that argument LUNIT is not changed. Interfaces of all BIEF subroutines have been put in a single module called BIEF. a `USE BIEF` statement at the beginning of a subroutine will prompt the compiler to check the arguments and also do some optimisations in view of the `INTENT` information (which can be `IN`, `OUT`, or `INOUT` depending on the use of the argument). If a function is declared in an interface, it must not be declared as an `EXTERNAL FUNCTION`.

4.1.5 Interface operator

New operations on structures could also be defined with the `INTERFACE OPERATOR` statement. For example a sum of two vectors as stored in BIEF could be defined so that the line:

```
CALL OS('X=Y     ',U,V,V,0.D0)
```

could be replaced by:

```
U=V
```

Such interface operators **have not been done** in this code , because operations like U=A+B+C would probably not be optimised and would trigger a number of unnecessary copies.

4.1.6 Optional parameters

Subroutines may now have optional parameters. Thanks to this new feature, subroutines OS and OSD of previous releases have been grouped in a single one. Hereafter is given the interface of new subroutine OS:

```
INTERFACE
SUBROUTINE OS( OP, X , Y , Z , C , IOPT , INFINI , ZERO )
 USE BIEF_DEF
 INTEGER, INTENT(IN), OPTIONAL :: IOPT
 DOUBLE PRECISION, INTENT(IN), OPTIONAL, INFINI, ZERO
 TYPE(BIEF_OBJ), INTENT(INOUT), OPTIONAL :: X
 TYPE(BIEF_OBJ), INTENT(IN), OPTIONAL :: Y,Z
 DOUBLE PRECISION, INTENT(IN), OPTIONAL :: C
 CHARACTER(LEN=8), INTENT(IN) :: OP
END SUBROUTINE

END INTERFACE
```

Subroutine OS performs on structure X the operation given in OP, e.g.

```
CALL OS('X=0     ',X=TRA01)
```

Or:

```
CALL OS('X=Y     ',X=TAB1,Y=TAB2)
```

Parameters Y,Z and C are used only for specific operations and otherwise are not necessary. When a parameter is missing and to avoid ambiguity, the parameters must be named, hence the X=TRA01 in the example above.
Parameters IOPT, INFINI and ZERO stem from the old subroutine OSD and are used only when a division is implied in the operation asked, for example if OP = 'X=Y/Z '. These 3 parameters are now optional. When they are present, it is better to name them as is done in the following line:

```
CALL OS('X=Y/Z   ',U,V,W,0.D0,IOPT=2,INFINI=1.D0,ZERO=1.D-10)
```

The use of optional parameters will enable a better compatibility between different versions because it will be possible to add a new parameter as an optional one.
Optional arguments will be written between brackets [ ] in argument lists in the rest of the document.

4.2 Structures in BIEF

4.2.1 A short description

In BIEF structures will be composed of integer and real numbers, of pointers to other structures or to integer and real arrays. The structures defined in this way are, for the time being, as follows:

- BIEF_OBJ (may be a vector, a matrix or a block)

- BIEF_MESH (information on a mesh)
- SLVCFG (Solver Configuration)
- BIEF_FILE (Description of a data file)

The notions of `VECTOR`, `MATRIX` and `BLOCK` that were pre-programmed in BIEF 6.2 have been gathered in a single structure called `BIEF_OBJ`. This will enable what is called "polymorphism" in Object Oriented Languages, i.e. the fact that arguments of subroutines may be of different types. As a matter of fact, many subroutines in BIEF are able to treat in the same way vectors or blocks of vectors (see for example OS), matrices or blocks of matrices (see e.g. `SOLVE` and `DIRICH`). Polymorphism is possible in FORTRAN 90 with the use of interfaces, however it requires the writing of one subroutine per combination of types, and thus leads to a lot of duplication. The use of a single structure `BIEF_OBJ` was thus more elegant, the only drawback being that the misuse of a matrix as a vector, for example, cannot be checked by the compiler but only by the subroutines dealing with such structures.
Information on the structures can be simply retrieved by the component selector.
We shall also refer to `BIEF_OBJ` structures as `VECTOR`, `MATRIX` or `BLOCK`, depending on their use, as is done below:

VECTOR

This may be any vector (a simple array) or a vector defined on the mesh, with values for every point of the mesh. In the latter case, there is a corresponding discretisation type and numbering system (global or boundary numbering of nodes or numbering of elements). For example, a vector defined on all the mesh with a discretisation P0 will be implicitly given according to the element numbers. In certain conditions, a vector may change discretisation while the calculations are being carried out.
A vector has a first dimension which corresponds to the number of nodes to which it applies. There is also a second dimension (for example, the off-diagonal terms of a matrix).
Any vector is in fact an array with 2 dimensions which the user can process as he wishes.

MATRIX

Matrices are also linked to the mesh. Different storage methods are possible. These matrices can be multiplied by the vectors mentioned above.

BLOCK

A block is a set of structures. This notion has proved of particular importance for:

- Writing general solvers for linear systems, with the possibility of the matrix being a block of several matrices.
- Using simple orders to group together and process sets of vectors or matrices, for example the arrays of variables which are advected by the method of characteristics.
- Eliminate the need for certain arrays to follow one another in the memory.

`BIEF_MESH` structure

This structure includes all information concerning the mesh (connectivity tables, boundary points, point coordinates, etc.). It replaces a large number of arrays used in releases of BIEF prior to 3.2

SLVCFG

It stands for "SoLVer ConFiGuration). This is a simple structure to store all the information needed by the subroutine SOLVE for solving linear systems (choice of the method, accuracy, preconditioning, etc).

4.2.2 Reference description of the structures

Module BIEF_DEF of the library is given hereafter, with the list of components for every structure and a short description.

POINTER_TO_BIEF_OBJ

```
!
!=====================================================================
!
!  STRUCTURE OF POINTER TO A BIEF_OBJ, TO HAVE ARRAYS OF POINTERS
!  IN THE BIEF_OBJ STRUCTURE FOR BLOCKS
!
!  BIEF VERSION 6.0
!
!=====================================================================
!
!       THIS IS NECESSARY IN FORTRAN 90 TO HAVE ARRAYS OF POINTERS
!       LIKE THE COMPONENT ADR BELOW, WHICH ENABLES TO BUILD BLOCKS
!       WHICH ARE ARRAYS OF POINTERS TO BIEF_OBJ STRUCTURES
!
        TYPE POINTER_TO_BIEF_OBJ
          SEQUENCE
          TYPE(BIEF_OBJ), POINTER :: P
        END TYPE POINTER_TO_BIEF_OBJ
```

BIEF_OBJ

```
        TYPE BIEF_OBJ
!
!---------------------------------------------------------------------
!
!       HEADER COMMON TO ALL OBJECTS
!
!         KEY : ALWAYS 123456 TO CHECK MEMORY OVERWRITING
          INTEGER KEY
!
!         TYPE: 2: VECTOR,   3: MATRIX,   4: BLOCK
          INTEGER TYPE
!
!         NAME: FORTRAN NAME OF OBJECT IN 6 CHARACTERS
          CHARACTER(LEN=6) NAME
!
!---------------------------------------------------------------------
!
!       FOR VECTORS
!
!         NAT: NATURE (1:DOUBLE PRECISION  2:INTEGER)
          INTEGER NAT
!
!         ELM: TYPE OF ELEMENT
          INTEGER ELM
```

```
!
!          DIM1: FIRST DIMENSION OF VECTOR
           INTEGER DIM1
!
!          MAXDIM1: MAXIMUM SIZE PER DIMENSION
           INTEGER MAXDIM1
!
!          DIM2: SECOND DIMENSION OF VECTOR
           INTEGER DIM2
!
!          MAXDIM2: MAXIMUM SECOND DIMENSION OF VECTOR
           INTEGER MAXDIM2
!
!          DIMDISC: TYPE OF ELEMENT IF VECTOR IS DISCONTINUOUS AT
!                   THE BORDER BETWEEN ELEMENTS, OR 0 IF NOT
           INTEGER DIMDISC
!
!          STATUS:
!          0: ANY ARRAY
!          1: VECTOR DEFINED ON A MESH, NO CHANGE OF DISCRETISATION
!          2: VECTOR DEFINED ON A MESH, CHANGE
!                          OF DISCRETISATION ALLOWED
           INTEGER STATUS
!
!          TYPR: TYPE OF VECTOR OF REALS
!          '0' : NIL   '1' : EQUAL TO 1  'Q' : NO SPECIFIC PROPERTY
           CHARACTER*1 TYPR
!
!          TYPR: TYPE OF VECTOR OF REALS
!          '0' : NIL   '1' : EQUAL TO 1  'Q' : NO SPECIFIC PROPERTY
           CHARACTER*1 TYPI
!
!          POINTER TO DOUBLE PRECISION 1-DIMENSION ARRAY
!          DATA ARE STORED HERE FOR A DOUBLE PRECISION VECTOR
           DOUBLE PRECISION, POINTER,DIMENSION(:)::R
!
!          POINTER TO INTEGER 1-DIMENSION ARRAY
!          DATA ARE STORED HERE FOR AN INTEGER VECTOR
           INTEGER, POINTER,DIMENSION(:)::I
!
!---------------------------------------------------------------------
!
!        FOR MATRICES
!
!          STO: TYPE OF STORAGE 1: CLASSICAL EBE 3: EDGE-BASED STORAGE
           INTEGER STO
!
!          ELMLIN: TYPE OF ELEMENT OF LINE
           INTEGER ELMLIN
!
!          ELMCOL: TYPE OF ELEMENT OF COLON
           INTEGER ELMCOL
!
!          TYPDIA: TYPE OF DIAGONAL
!          '0' : NIL   'I' : IDENTITY  'Q' : NO SPECIFIC PROPERTY
           CHARACTER*1 TYPDIA
```

```
!
!          TYPEXT: TYPE OF EXTRA-DIAGONAL TERMS
!          '0' : NIL   'S' : SYMMETRY  'Q' : NO SPECIFIC PROPERTY
           CHARACTER*1 TYPEXT
!
!          POINTER TO A BIEF_OBJ FOR DIAGONAL
           TYPE(BIEF_OBJ), POINTER :: D
!
!          POINTER TO A BIEF_OBJ FOR EXTRA-DIAGONAL TERMS
           TYPE(BIEF_OBJ), POINTER :: X
!
!          PRO: TYPE OF MATRIX-VECTOR PRODUCT
           INTEGER PRO
!
!--------------------------------------------------------------------
!
!       FOR BLOCKS
!
!         BLOCKS ARE IN FACT ARRAYS OF POINTERS TO BIEF_OBJ
!         STRUCTURES ADR(I)\%P WILL BE THE I-TH BIEF_OBJ OBJECT
!
!         N: NUMBER OF OBJECTS IN THE BLOCK
          INTEGER N
!         MAXBLOCK: MAXIMUM NUMBER OF OBJECTS IN THE BLOCK
          INTEGER MAXBLOCK
!         ADR: ARRAY OF POINTERS TO OBJECTS (WILL BE OF SIZE MAXBLOCK)
          TYPE(POINTER_TO_BIEF_OBJ), POINTER, DIMENSION(:) :: ADR
!
!--------------------------------------------------------------------
!
        END TYPE BIEF_OBJ
!
!====================================================================
!
```

BIEF_MESH

```
!
!====================================================================
!
!   STRUCTURE OF MESH : BIEF_MESH
!
!====================================================================
!
      TYPE BIEF_MESH
!
!        1) A HEADER
!
!        NAME: NAME OF MESH IN 6 CHARACTERS
         CHARACTER(LEN=6) NAME
!
!        2) A SERIES OF INTEGER VALUES (DECLARED AS POINTERS TO ENABLE
!                                       ALIASES)
!
!        NELEM: NUMBER OF ELEMENTS IN MESH
         INTEGER, POINTER :: NELEM
!
```

```
!        NELMAX: MAXIMUM NUMBER OF ELEMENTS ENVISAGED
         INTEGER, POINTER :: NELMAX
!
!        NPTFR: NUMBER OF 1D BOUNDARY NODES, EVEN IN 3D
         INTEGER, POINTER :: NPTFR
!
!        NPTFRX: NUMBER OF 1D BOUNDARY NODES, EVEN IN 3D
         INTEGER, POINTER :: NPTFRX
!
!        NELEB: NUMBER OF BOUNDARY ELEMENTS (SEGMENTS IN 2D)
!        IN 3D WITH PRISMS:
!        number of LATERAL boundary elements for sigma mesh
         INTEGER, POINTER :: NELEB
!
!        NELEBX: MAXIMUM NELEB
         INTEGER, POINTER :: NELEBX
!
!        NSEG: NUMBER OF SEGMENTS IN THE MESH
         INTEGER, POINTER :: NSEG
!
!        DIM: DIMENSION OF DOMAIN (2 OR 3)
         INTEGER, POINTER :: DIM
!
!        TYPELM: TYPE OF ELEMENT (10 FOR TRIANGLES, 40 FOR PRISMS)
         INTEGER, POINTER :: TYPELM
!
!        NPOIN: NUMBER OF VERTICES (OR LINEAR NODES) IN THE MESH
         INTEGER, POINTER :: NPOIN
!
!        NPMAX: MAXIMUM NUMBER OF VERTICES IN THE MESH
         INTEGER, POINTER :: NPMAX
!
!        MXPTVS: MAXIMUM NUMBER OF POINTS ADJACENT TO 1 POINT
         INTEGER, POINTER :: MXPTVS
!
!        MXELVS: MAXIMUM NUMBER OF ELEMENTS ADJACENT TO 1 POINT
         INTEGER, POINTER :: MXELVS
!
!        LV: MAXIMUM VECTOR LENGTH ALLOWED ON VECTOR COMPUTERS,
!            DUE TO ELEMENT NUMBERING
         INTEGER, POINTER :: LV
!
!
!        3) A SERIES OF BIEF_OBJ FOR STORING INTEGER ARRAYS
!
!        IKLE: CONNECTIVITY TABLE IKLE(NELMAX,NDP)
!              AND KLEI(NDP,NELMAX)
         TYPE(BIEF_OBJ), POINTER :: IKLE,KLEI
!
!        IFABOR: TABLE GIVING ELEMENTS BEHIND FACES OF A TRIANGLE
         TYPE(BIEF_OBJ), POINTER :: IFABOR
!
!        NELBOR: ELEMENTS OF THE BORDER
         TYPE(BIEF_OBJ), POINTER :: NELBOR
!
!        NULONE: LOCAL NUMBER OF BOUNDARY POINTS FOR BORDER ELEMENTS
```

```
        TYPE(BIEF_OBJ), POINTER :: NULONE
!
!       KP1BOR: POINTS FOLLOWING AND PRECEDING A BOUNDARY POINT
        TYPE(BIEF_OBJ), POINTER :: KP1BOR
!
!       NBOR: GLOBAL NUMBER OF BOUNDARY POINTS
        TYPE(BIEF_OBJ), POINTER :: NBOR
!
!       IKLBOR: CONNECTIVITY TABLE FOR BOUNDARY POINTS
        TYPE(BIEF_OBJ), POINTER :: IKLBOR
!
!       IFANUM: FOR STORAGE 2, NUMBER OF SEGMENT IN ADJACENT ELEMENT
!       OF A TRIANGLE
        TYPE(BIEF_OBJ), POINTER :: IFANUM
!
!       IKLEM1: ADRESSES OF NEIGHBOURS OF POINTS FOR FRONTAL
!       MATRIX-VECTOR PRODUCT
        TYPE(BIEF_OBJ), POINTER :: IKLEM1
!
!       LIMVOI: FOR FRONTAL MATRIX-VECTOR PRODUCT.
!       ADDRESSES OF POINTS WITH A GIVEN NUMBER OF NEIGHBOURS.
        TYPE(BIEF_OBJ), POINTER :: LIMVOI
!
!       NUBO: FOR FINITE VOLUMES,
!             GLOBAL NUMBERS OF VERTICES OF SEGMENTS
        TYPE(BIEF_OBJ), POINTER :: NUBO
!
!       FOR SEGMENT-BASED STORAGE
!
!       GLOSEG: GLOBAL NUMBERS OF VERTICES OF SEGMENTS
        TYPE(BIEF_OBJ), POINTER :: GLOSEG
!       ELTSEG: SEGMENTS FORMING AN ELEMENT
        TYPE(BIEF_OBJ), POINTER :: ELTSEG
!       ORISEG: ORIENTATION OF SEGMENTS FORMING AN ELEMENT
!               1:TRIGO 2:CLOCKWISE
        TYPE(BIEF_OBJ), POINTER :: ORISEG
!
!
!       SERIES OF ARRAYS FOR PARALLELISM
!       HERE GLOBAL MEANS NUMBER IN THE WHOLE DOMAIN
!            LOCAL  MEANS NUMBER IN THE SUB-DOMAIN
!
!       KNOLG: GIVES THE INITIAL GLOBAL NUMBER OF A LOCAL POINT
        TYPE(BIEF_OBJ), POINTER :: KNOLG
!       NACHB: NUMBERS OF PROCESSORS CONTAINING A GIVEN POINT
        TYPE(BIEF_OBJ), POINTER :: NACHB
!       ISEG: GLOBAL NUMBER OF FOLLOWING OR PRECEDING POINT
!             IN THE BOUNDARY
!       IF IT IS IN ANOTHER SUB-DOMAIN.
        TYPE(BIEF_OBJ), POINTER :: ISEG
!       KNOGL: INVERSE OF KNOLG, KNOGL(KNOLG(I))=I. LOCAL NUMBER OF A
!       POINT WITH GIVEN GLOBAL NUMBER
        TYPE(BIEF_OBJ), POINTER :: KNOGL
!       ADDRESSES IN ARRAYS SENT BETWEEN PROCESSORS
        TYPE(BIEF_OBJ), POINTER :: INDPU
!
```

```
!         DIMENSION NHP(NBMAXNSHARE,NPTIR).
!         NHP(IZH,IR) IS THE GLOBAL NUMBER
!         IN THE SUB-DOMAIN OF A POINT WHOSE NUMBER IS IR
!         IN THE INTERFACE
!         WITH THE IZ-TH HIGHER RANK PROCESSOR
          TYPE(BIEF_OBJ), POINTER :: NHP
!         NHM IS LIKE NHP, BUT WITH LOWER RANK PROCESSORS
          TYPE(BIEF_OBJ), POINTER :: NHM
!
!         FOR FINITE VOLUMES AND KINETIC SCHEMES
          TYPE(BIEF_OBJ), POINTER :: JMI
!         ELEMENTAL HALO NEIGHBOURHOOD DESCRIPTION IN PARALLEL
!         IFAPAR(6,NELEM2)
!         IFAPAR(1:3,IELEM):
!                   PROCESSOR NUMBERS BEHIND THE 3 ELEMENT EDGES
!                   NUMBER FROM 0 TO NCSIZE-1
!         IFAPAR(4:6,IELEM):
                    -LOCAL- ELEMENT NUMBERS BEHIND THE 3 EDGES
!                  IN THE NUMBERING OF PARTITIONS THEY BELONG TO
          TYPE(BIEF_OBJ), POINTER :: IFAPAR
!
!         4) A SERIES OF BIEF_OBJ FOR STORING REAL ARRAYS
!
!         XEL: COORDONNEES X PAR ELEMENTS
          TYPE(BIEF_OBJ), POINTER :: XEL
!
!         YEL: COORDONNEES Y PAR ELEMENTS
          TYPE(BIEF_OBJ), POINTER :: YEL
!
!         ZEL: COORDONNEES Z PAR ELEMENTS
          TYPE(BIEF_OBJ), POINTER :: ZEL
!
!         SURFAC: AREAS OF ELEMENTS
          TYPE(BIEF_OBJ), POINTER :: SURFAC
!
!         SURDET: 1/DET OF ISOPARAMETRIC TRANSFORMATION
          TYPE(BIEF_OBJ), POINTER :: SURDET
!
!         LGSEG: LENGTH OF 2D BOUNDARY SEGMENTS
          TYPE(BIEF_OBJ), POINTER :: LGSEG
!
!         XSGBOR: NORMAL X TO 1D BOUNDARY SEGMENTS
          TYPE(BIEF_OBJ), POINTER :: XSGBOR
!
!         YSGBOR: NORMAL Y TO 1D BOUNDARY SEGMENTS
          TYPE(BIEF_OBJ), POINTER :: YSGBOR
!
!         ZSGBOR: NORMAL Z TO 1D BOUNDARY SEGMENTS
          TYPE(BIEF_OBJ), POINTER :: ZSGBOR
!
!         XNEBOR: NORMAL X TO 1D BOUNDARY POINTS
          TYPE(BIEF_OBJ), POINTER :: XNEBOR
!
!         YNEBOR: NORMAL Y TO 1D BOUNDARY POINTS
          TYPE(BIEF_OBJ), POINTER :: YNEBOR
!
```

```
!        ZNEBOR: NORMAL Z TO 1D BOUNDARY POINTS
         TYPE(BIEF_OBJ), POINTER :: ZNEBOR
!
!        X: COORDINATES OF POINTS
         TYPE(BIEF_OBJ), POINTER :: X
!
!        Y: COORDINATES OF POINTS
         TYPE(BIEF_OBJ), POINTER :: Y
!
!        Z: COORDINATES OF POINTS
         TYPE(BIEF_OBJ), POINTER :: Z
!
!        COSLAT: LATITUDE COSINE
         TYPE(BIEF_OBJ), POINTER :: COSLAT
!
!        SINLAT: LATITUDE SINE
         TYPE(BIEF_OBJ), POINTER :: SINLAT
!
!        DISBOR: DISTANCE TO 1D BOUNDARIES
         TYPE(BIEF_OBJ), POINTER :: DISBOR
!
!        M: WORKING MATRIX
         TYPE(BIEF_OBJ), POINTER :: M
!
!        MSEG: WORKING MATRIX FOR SEGMENT-BASED STORAGE
         TYPE(BIEF_OBJ), POINTER :: MSEG
!
!        W: WORKING ARRAY FOR A NON-ASSEMBLED VECTOR
         TYPE(BIEF_OBJ), POINTER :: W
!
!        T: WORKING ARRAY FOR AN ASSEMBLED VECTOR
         TYPE(BIEF_OBJ), POINTER :: T
!
!        VNOIN: FOR FINITE VOLUMES
         TYPE(BIEF_OBJ), POINTER :: VNOIN
!
!        XSEG: X COORDINATE OF FOLLOWING
!              OR PRECEDING POINT IN THE BOUNDARY
!        IF IT IS IN ANOTHER SUB-DOMAIN.
         TYPE(BIEF_OBJ), POINTER :: XSEG
!
!        YSEG: Y COORDINATE OF FOLLOWING
!              OR PRECEDING POINT IN THE BOUNDARY
!        IF IT IS IN ANOTHER SUB-DOMAIN.
         TYPE(BIEF_OBJ), POINTER :: YSEG
!
!        FAC: MULTIPLICATION FACTOR FOR POINTS IN THE BOUNDARY FOR
!             DOT PRODUCT.
         TYPE(BIEF_OBJ), POINTER :: FAC
!
!        FOR PARALLELISM AND NON BLOCKING COMMUNICATION (SEE PARINI.F)
!
!        NUMBER OF NEIGHBOURING PROCESSORS (SEEN BY POINTS)
         INTEGER        , POINTER :: NB_NEIGHB
!        FOR ANY NEIGHBOURING PROCESSOR, NUMBER OF POINTS
!        SHARED WITH IT
```

```
        TYPE(BIEF_OBJ), POINTER :: NB_NEIGHB_PT
!       RANK OF PROCESSORS WITH WHICH TO COMMUNICATE FOR POINTS
        TYPE(BIEF_OBJ), POINTER :: LIST_SEND
!       NH_COM(DIM1NHCOM,NB_NEIGHB)
!       WITH DIM1NHCOM IS THE MAXIMUM NUMBER OF POINTS SHARED
!       WITH ANOTHER PROCESSOR
!       (OR SLIGHTLY MORE FOR 16 BYTES ALIGNMENT)
!       NH_COM(I,J) IS THE GLOBAL NUMBER IN THE SUB-DOMAIN OF I-TH
!       POINT SHARED WITH J-TH NEIGHBOURING PROCESSOR
        TYPE(BIEF_OBJ), POINTER :: NH_COM
!
!       NUMBER OF NEIGHBOURING PROCESSORS (SEEN BY EDGES)
        INTEGER       , POINTER :: NB_NEIGHB_SEG
!       FOR ANY NEIGHBOURING PROCESSOR, NUMBER OF EDGES
!       SHARED WITH IT
        TYPE(BIEF_OBJ), POINTER :: NB_NEIGHB_PT_SEG
!       RANK OF PROCESSORS WITH WHICH TO COMMUNICATE FOR EDGES
        TYPE(BIEF_OBJ), POINTER :: LIST_SEND_SEG
!       LIKE NH_COM BUT FOR EDGES
        TYPE(BIEF_OBJ), POINTER :: NH_COM_SEG
!
!       WILL BE USED AS BUFFER BY MPI IN PARALLEL
!
        TYPE(BIEF_OBJ), POINTER :: BUF_SEND
        TYPE(BIEF_OBJ), POINTER :: BUF_RECVC
!       FOR FINITE VOLUMES AND KINETIC SCHEMES
!
        TYPE(BIEF_OBJ), POINTER :: CMI,DPX,DPY
        TYPE(BIEF_OBJ), POINTER :: DTHAUT,AIRST
!
      END TYPE BIEF_MESH
!
!=====================================================================
!
```

SLVCFG

```
!
!=====================================================================
!
!  STRUCTURE OF SOLVER CONFIGURATION
!
!=====================================================================
!
        TYPE SLVCFG
!
!         SLV: CHOICE OF SOLVER
          INTEGER SLV
!
!         NITMAX: MAXIMUM NUMBER OF ITERATIONS
          INTEGER NITMAX
!
!         PRECON: TYPE OF PRECONDITIONING
          INTEGER PRECON
!
!         KRYLOV: DIMENSION OF KRYLOV SPACE FOR GMRES SOLVER
          INTEGER KRYLOV
```

```
!
!          EPS: ACCURACY
           DOUBLE PRECISION EPS
!
!          ZERO: FOR CHECKING DIVISIONS BY ZERO
           DOUBLE PRECISION ZERO
!
!          OK: IF PRECISION EPS HAS BEEN REACHED
           LOGICAL OK
!
!          NIT: NUMBER OF ITERATIONS IF PRECISION REACHED
           INTEGER NIT
!
         END TYPE SLVCFG
!
!=====================================================================
!
```

BIEF_FILE

```
!
!=====================================================================
!
!  STRUCTURE OF FILE
!
!=====================================================================
!
         TYPE BIEF_FILE
!
!          LU: LOGICAL UNIT TO OPEN THE FILE
           INTEGER LU
!
!          NAME: NAME OF FILE
           CHARACTER(LEN=144) NAME
!
!          TELNAME: NAME OF FILE IN TEMPORARY DIRECTORY
           CHARACTER(LEN=6) TELNAME
!
!          FMT: FORMAT (SERAFIN, MED, ETC.)
           CHARACTER(LEN=8) FMT
!
!          ACTION: READ, WRITE OR READWRITE
           CHARACTER(LEN=9) ACTION
!
!          BINASC: ASC FOR ASCII OR BIN FOR BINARY
           CHARACTER(LEN=3) BINASC
!
!          TYPE: KIND OF FILE
           CHARACTER(LEN=12) TYPE
!
         END TYPE BIEF_FILE
```

4.2.3 Allocation of structures

Once declared, `BIEF_OBJ` structures must be defined and memory for their arrays of data must be dynamically allocated. This is done by specific subroutines, depending of their type, i.e. whether they are vectors, matrices or blocks. `BIEF_MESH` structure must also be allocated.

The allocations of structures are grouped in a subroutine called POINT_NAME (NAME is the name of a TELEMAC-MASCARET SYSTEM program, for example ARTEMIS).
The mesh structure must be allocated first. Vectors and matrices will then be allocated with respect to that mesh.

Mesh: subroutine ALMESH

A mesh must be declared previously as a BIEF_MESH structure
Syntax:

```
CALL ALMESH( MESH, NOM, IELM, SPHERI,CFG,NFIC,
             EQUA,NPLAN,NPMAX,NPTFRX,NELMAX,I3,I4)
```

ALMESH prepares the BIEF_MESH structures and fills some of them, for example it will allocate the memory for storing the component IKLE and will read it in the geometry file. However not all the data structure is ready after exiting ALMESH. This task is carried out by the subroutine INBIEF which must be called later, when all the necessary data have been logged.
Arguments:

MESH The BIEF_MESH structure to allocate.

NOM Fortran name of this structure in 6 characters.

IELM Element with the highest number of degrees of freedom in the mesh.

- **11** only linear interpolation in 2D
- **12** quasi-bubble in 2D
- **41** linear in 3D with prisms

SPHERI Logical. If true, coordinates will be spherical, if not, Cartesian.

CFG Configuration. So far 2 integer values:

- **CFG(1)** is the storage of matrices (1: classical EBE, 3: edge-based)
- **CFG(2)** is the matrix-vector product (1: classical EBE, 2: frontal)

These data will be used to build specific data structures relevant to every option.

NFIC Logical unit where the geometry file has been opened.

EQUA Equations to solve or calling programme in 20 characters. Up to now is only used to allocate specific arrays for Finite volumes if EQUA='SAINT-VENANT VF' is used to optimise memory requirements.

Next 6 arguments are optional:

NPLAN Number of horizontal planes in 3D meshes of prisms.

NPMAX Maximum number of vertices in the mesh, in case of adaptive meshing (not implemented yet).

NPTFRX Maximum number of boundary points in the mesh, in case of adaptive meshing (not implemented yet).

NELMAX Maximum number of elements in the mesh, in case of adaptive meshing (not implemented yet).

I3, I4 When present, it means that the X and Y coordinates of the mesh are in reality X+I3 and Y+I4, I3 and I4 (integers representing a number of metres, have been removed to minimize truncation errors (see also the Selafin format where these two numbers are included for a geo-referenced post-processing.

Vector : BIEF_ALLVEC , BIEF_ALLVEC_IN_BLOCK
A vector must be declared previously as a `BIEF_OBJ` structure
Syntax:

```
CALL BIEF_ALLVEC(NAT,VEC,NOM,IELM,DIM2,STATUT,MESH)
```

Arguments:

NAT Nature (1=real, 2=integer).

VEC The BIEF_OBJ structure to be allocated as a vector.

NOM Fortran name of vector in 6 characters.

IELM Vector discretisation type (**or dimension depending on the status**, **see below**)

- **0** dimension 1, constant per element.
- **1** dimension 1 linear discretisation.
- **10** triangles, constant discretisation per element.
- **11** triangles, linear discretisation.
- **12** triangles, quasi-bubble discretisation.
- **40** prism, constant discretisation per element.
- **41** prism, linear discretisation.

DIM2 Second dimension of vector.

STATUT **0** Any array. **IELM is then its first dimension**.

- **1** Vector defined on a mesh, with no possibility of changing discretisation.
- **2** Vector defined on a mesh, with possibility of changing discretisation within the limits of the memory space.

MESH the BIEF_MESH structure with data on the mesh.

Syntax:

```
CALL BIEF_ALLVEC_IN_BLOCK( BLO,N,NAT,NOM,IELM,DIM2,STATUT)
```

With `BIEF_ALLVEC_IN_BLOCK`, N vectors with the same characteristics are put directly into the block BLO. NOM is then only a generic name, for example if NOM is 'T ', the names of the vectors will be T1, T2, etc. Only the block BLO must be declared. T2 will be in fact BLO%ADR(2)%P but can be named also T2 if T2 is declared as a `BIEF_OBJ` pointer and pointed to BLO%ADR(2)%P:

```
TYPE(BIEF_OBJ), POINTER :: T2
T2 => BLO%ADR(2)%P
```

Matrix: BIEF_ALLMAT

A matrix must be declared previously as a BIEF_OBJ structure. We only deal with matrices of double precision numbers.
Syntax:

```
CALL BIEF_ALLMAT( MAT,NOM,IELM1,IELM2,
CFG,TYPDIA,TYPEXT,MESH)
```

Arguments:

MAT The BIEF_OBJ structure to be allocated as a vector.

NOM Fortran name of matrix in 6 characters.

IELM1 Type of discretisation for rows (same convention as for the vectors).

IELM2 Type of discretisation for columns.

CFG Configuration. So far 2 integer values:

- CFG(1) is the storage of matrices (1: EBE, 3: edge based)
- CFG(2) is the matrix-vector product (1: EBE, 2: frontal)

TYPDIA Diagonal type ('0' : zero, 'Q' : any, 'I' : identity)

TYPEXT Type of the off-diagonal terms ('0': zero, 'Q': any, 'S': symmetrical)

MESH : Bief_mesh structure with data on the mesh.

Block : ALLBLO

A block must be declared previously as a BIEF_OBJ structure.
Syntax:

```
CALL ALLBLO(BLO,NOM)
```

Arguments:

BLO The BIEF_OBJ structure to be allocated as a block.

NOM Fortran name of block in 6 characters.

In this case, we have an empty shell where we do not specify which objects have been placed in the block. A block structure can thus be used again. To fill the block, the subroutine ADDBLO must then be called (see paragraph A.I.4.4). The syntax will be:

```
CALL ADDBLO(BLOCK,OBJ)
```

to add a BIEF_OBJ structure OBJ to the block called BLOCK.
A block can be emptied by calling a simple function:

```
CALL DEALLBLO(BLOCK)
```

Example

We take here the example of a double precision array called SAMPLE, with one dimension, and quasi-bubble discretisation. This vector will be then set to a constant value.

1. Declare the structure:

   ```
   TYPE(BIEF_OBJ) :: SAMPLE
   ```

   in a global declaration through a module, or locally.

2. Allocate the structure:

   ```
   CALL BIEF_ALLVEC(1,SAMPLE,'SAMPLE',12,1,STATUT,MESH)
   ```

3. To set the value of the vector to 5.D0 for all points of the mesh, you can then do:

   ```
   CALL OS('X=C     ',X=SAMPLE,C=5.D0)
   ```

   which is equivalent in this case to (but the following would require declaration of integer I):

   ```
   DO I=1,SAMPLE%DIM1
      SAMPLE%R(I)=5.D0
   ENDDO
   ```

To understand this loop, remember that R is the component storing the real data of vectors, and DIM1 the size of the first dimension. However it is not mandatory to remember this if you use the functions and subroutines designed for operations on structures.

4.2.4 Operations on structures

The functions and subroutines described below are used for manipulating structures without having to know how they are arranged. This paragraph will be limited to the functions related to the notion of structure itself. The traditional operations on matrices and vectors will be dealt with in Chapter 4.3.
All the functions described hereafter will be naturally declared by a USE BIEF statement at the beginning of subroutines. Otherwise they would have to be declared as EXTERNAL.

General operations on structures

syntax:

```
LOGICAL FUNCTION CMPOBJ(T1,T2)
```

arguments:

T1,T2 a vector or a block

`CMPOBJ` indicates if the two structures are identical. A check is made to see whether these two structures are of the same type and, if so, their characteristics are compared:

- for vectors: discretisation.
- for blocks: the number of structures that it contains.

Nothing has been done so far for the other structures.
This function is used by subroutine OS.

Operations on vectors

syntax:

```
SUBROUTINE CHGDIS(VEC,OLDELT,NEWELT,MESH)
```

CHGDIS changes the discretisation of a vector.
arguments:

VEC is the vector

MESH the structure containing the mesh integers

OLDELT is the former vector discretisation

NEWELT is the new one

A vector can thus go from a linear discretisation to a quasi-bubble discretisation, or the reverse. In the first case, the missing values are found by linear interpolation, while in the second case the superfluous values are forgotten. There are certain restrictions to the use of this subroutine:

- a vector cannot be extended if the required memory space is not provided for during allocation.
- Certain changes are impossible, for obvious reasons: changing a triangle to a quadrilateral, etc.

syntax:

```
SUBROUTINE CPSTVC(T1,T2)
```

This subroutine copies a vector structure onto another. If T1 is a vector, T2 then becomes a vector with the same characteristics. Nevertheless, the memory allocated during allocation cannot be changed. The only data copied for the moment are:

- Discretisation type (component ELM)
- The first dimension (component DIM1)
- The second dimension (component DIM2)
- The component DIMDISC in case of discontinuous vectors.

This subroutine should be used when dealing with temporary all purpose `BIEF_OBJ` structures like T1, T2, etc. in TELEMAC-2D and SISYPHE and T3_01, T3_02, etc. in TELEMAC-3D. As a matter of fact, these structures may have been changed by a previous use, e.g. they may have been turned into boundary vectors with a smaller size than a full domain vector, hence an initialisation like `CALL OS('X=0 ',X=T1)` may have a random effect if not secured previously by specifying what must be T1. Copying the structure of a known object like e.g. the depth in structure H, will do it. `CALL CPSTVC(H,T1)` will give T1 the same dimension and discretisation as the depth.

Operations on matrices

Note : all the operations on vectors may also be applied to the diagonal and the extradiagonal terms contained in the matrix structure (respectively `M%D` and `M%X` for a matrix M). The following subroutines only apply to matrices:
syntax:

```
SUBROUTINE CPSTMT(M1,M2,TRANS)
```

Copies characteristics of the matrix M1 on to the matrix M2, or of transposed of matrix M1 to M2 (if optional argument TRANS is set to true).
`CPSTMT` is similar to `CPSTVC`, it carries out the following operations:

1. copies types of elements.
2. copies types of diagonal and off-diagonal terms (calls CPSTVC for the diagonal and the off-diagonal terms).
3. copies characteristics of the matrix (components TYPDIA and TYPEXT).
4. checks that M2 has enough memory for its new characteristics : sizes of diagonal and extra-diagonal terms.

syntax:

```
INTEGER FUNCTION BIEF_DIM1_EXT(IELM1,IELM2,STO,TYPEXT,MESH)
```

The extra-diagonal terms of matrices are stored in 2-dimensional arrays. DIM1_EXT returns the first dimension of this array, depending on: arguments:

IELM1 Type of discretisation for rows (same convention as for the vectors).

IELM2 Type of discretisation for columns.

STO : Storage of the matrix (1: EBE, 3: edge based)

TYPEXT Type of the off-diagonal terms ('0': zero, 'Q': any, 'S': symmetrical)

MESH `BIEF_MESH` structure with data on the mesh.

syntax:

```
INTEGER FUNCTION BIEF_DIM2_EXT(IELM1,IELM2,STO,TYPEXT,MESH)
```

The extra-diagonal terms of matrices are stored in 2-dimensional arrays. `DIM2_EXT` returns the second dimension of this array, depending on: arguments:

IELM1 Type of discretisation for rows (same convention as for the vectors).

IELM2 Type of discretisation for columns.

STO Storage of the matrix (1: EBE, 3: edge based)

TYPEXT Type of the off-diagonal terms ('0': zero, 'Q': any, 'S': symmetrical)

MESH `BIEF_MESH` structure with data on the mesh.

Operations on blocks

syntax:

```
SUBROUTINE ADDBLO(BLOCK,T)
```

Adds the structure T to the block.
arguments:

BLOCK is a block

T a structure.

Reaching objects in blocks

If T1 is a vector stored as the second object in a block B, the address of T1 is B%ADR(2)%P. As a matter of fact, ADR is an array of `POINTER_TO_BIEF_OBJ` structures, we take the second one, and its unique component P (P would not be present if Fortran 90 were accepting the arrays of pointers).
`B%ADR(2)%P` can then be treated as a `BIEF_OBJ` structure, for example the third real value of T1 is `B%ADR(2)%P%R(3)`. It is not recommended to deal directly with objects in blocks, this can be done in a subroutine by calling it with the argument (e.g.) `B%ADR(2)%P`. It will be then received in the subroutine as a normal `BIEF_OBJ` structure.
Component selectors can be piled up if blocks themselves are stored in blocks as in the following example, where T1 as been stored as the second object into a block C stored as the third object in the block B. T1 is then:

```
B%ADR[3]%P%ADR[2]%P
```

The only difficulty and common error is to forget the component P which is due to Fortran obscure reasons.

4.3 Building matrices and vectors

The subroutines `MATRIX` and `VECTOR` construct matrices and vectors respectively, according to the instructions given in their arguments.

4.3.1 Construction of matrices

```
SUBROUTINE MATRIX( M,OP,FORMUL,IELM1,IELM2,
                   XMUL,F,G,H,U,V,W,MESH,MSK,MASKEL )
```

The result is the matrix M, with row element IELM1 and column element IELM2, constructed according to the formula FORMUL and the operation OP (see below). XMUL, F ,G ,H ,U ,V ,W are respectively a constant and six vector structures (defined with `TYPE(BIEF_OBJ)`) used in the definition of the matrix. The discretisation of F, G, H, U, V and W is checked and is taken into account in the calculations. These last six structures must not be dummy arguments, even if they are not used.
The other arguments are:
MESH Mesh declared as a BIEF_MESH structure.

MSK Logical. Indicates if the elements are masked.

MASKEL Element masking array.

Possible operations

OP is an operation coded in 8 characters, as for the subroutine OM. N is an internal working matrix which contains the matrix with the formula requested (see next paragraph). M is the matrix given by the user and which will be modified according to the operation indicated:

- OP = 'M=N ' : COPY OF N ON TO M
- OP = 'M=TN ' : COPY OF TRANSPOSED OF N ON TO M
- OP = 'M=M+N ' : N IS ADDED TO M
- OP = 'M=M+TN ' : TRANSPOSED OF N IS ADDED TO M

The operations with the form M=M+CN can be carried out through the multiplying factor XMUL which applies to N.

Available formulae

FORMUL is a string of 16 characters describing the formula. Generally only the first 6 are used but extra information may be contained in characters 7 to 16. For example the sixteenth character is sometimes used to specify the derivatives and may then contain the characters X, Y or Z.

Available elements

All the possible formulae are given below. However, all the discretisation combinations are not programmed. If a matrix or a given discretisation has not been programmed, an error message will appear to this effect.
In the next part of the text,Ψ_i is the base corresponding to the element IELM1 (row) and Ψ_j the base corresponding to the element IELM2 (column). The example of dimension 3 is given. For the other dimensions, some terms would of course have to be removed. The beginning of names of the corresponding subroutines in BIEF are given in brackets. They are complemented by letters indicating the elements treated. The first letter corresponds to the row and the second letter to the column. Letter O stands for a linear segment, A for a linear triangle, B for a quasi-bubble triangle, C for a quadratic triangle, P for a prism, T for a tetrahedron. More specifically F stands for a vertical linear triangle which is part of the vertical border of a mesh of prisms split into tetrahedrons. Example : subroutine MT01AA will compute the mass-matrix of a linear triangle.
<u>FORMUL = 'MATMAS '</u>
(in library BIEF subroutines with names which start with `MT01`)
Mass-matrix.

$$N(i,j) = XMUL \int_{\Omega} \Psi_i \Psi_j d\Omega$$

<u>FORMUL = 'MATDIF '</u>
(in library BIEF subroutines with names which start with `MT02`)
Diffusion matrix with different coefficients according to the directions x, y and z.
In 2 dimensions:

$$N(i,j) = XMUL \int_{\Omega} (U \frac{\partial \Psi_i}{\partial x} \frac{\partial \Psi_j}{\partial x} + U \frac{\partial \Psi_i}{\partial y} \frac{\partial \Psi_j}{\partial y}) d\Omega$$

The case of an isotropic viscosity is given above. But the viscosity may also be tensorial. In this case U (a `BIEF_OBJ` structure) must have a second dimension, for example 3 in 2-dimensional applications. U will has the general following form: $U = \begin{pmatrix} U_{xx} & U_{xy} \\ U_{yx} & U_{yy} \end{pmatrix}$, but the tensor is symmetric and Uxy = Uyx.
Elements of the tensor must be stored in U as follows:

- U_{xx} in U(*,1)
- U_{yy} in U(*,2)
- U_{xy} in U(*,3)

In a 2D non isotropic case, the diffusion matrix is of the form:

$$N(i,j) = XMUL \int_{\Omega} (U_{xx} \frac{\partial \Psi_i}{\partial x} \frac{\partial \Psi_j}{\partial x} + U_{yy} \frac{\partial \Psi_i}{\partial y} \frac{\partial \Psi_j}{\partial y} + U_{xy} \frac{\partial \Psi_i}{\partial x} \frac{\partial \Psi_j}{\partial y} + U_{xy} \frac{\partial \Psi_i}{\partial y} \frac{\partial \Psi_j}{\partial x}) d\Omega$$

When a transversal Kt and longitudinal Kl dispersion are used (case of Elder's turbulence model), the formula giving the tensor U is:

$$U_{xx} = Kl\cos(\theta)^2 + Kt\sin(\theta)^2$$

$$U_{yy} = Kl\sin(\theta)^2 + Kt\cos(\theta)^2$$

$$U_{xy} = (Kl - Kt)(\sin(\theta) - \cos(\theta))$$

In 3 dimensions (beware, F, G and H are used in this case, unlike in 2D where U,V and W are used):

$$N(i,j) = XMUL\int_\Omega (F\frac{\partial\Psi_i}{\partial x}\frac{\partial\Psi_j}{\partial x} + G\frac{\partial\Psi_i}{\partial y}\frac{\partial\Psi_j}{\partial y} + H\frac{\partial\Psi_i}{\partial z}\frac{\partial\Psi_j}{\partial z})d\Omega$$

FORMUL = 'MATDIF2 '
In 3D only, formula MATDIF2 is like `MATDIF`, but the hydrostatic inconsistencies are dealt with.
FORMUL = 'MATDIF3 '
In 2D only so far, diffusion matrix with diffusion coefficients which are piece-wise linear or constant, but may be discontinuous between elements (this is used in groundwater flows).

$$N(i,j) = XMUL\int_\Omega (U\frac{\partial\Psi_i}{\partial x}\frac{\partial\Psi_j}{\partial x} + V\frac{\partial\Psi_i}{\partial y}\frac{\partial\Psi_j}{\partial y})d\Omega$$

Here one must have:

```
U%ELM=10, U%DIM2=3, U%DIMDISC=11
V%ELM=10, V%DIM2=3, V%DIMDISC=11
```

FORMUL = 'MASUPG '
(subroutines with names which start with `MT03`)
Matrix used for the convection term with method SUPG option 1.

$$N(i,j) = XMUL\int_\Omega \boldsymbol{F}.\overrightarrow{grad}(\Psi_i)\boldsymbol{U}.\overrightarrow{grad}(\Psi_j)d\Omega$$

F here is a vector with the components F, G and H.
U is a vector with the components U, V and W.
FORMUL = 'MAUGUG '
(subroutines with names which start with `MT04`)
Matrix used for the convection term with method SUPG option 2.

$$N(i,j) = XMUL\int_\Omega \boldsymbol{U}.\overrightarrow{grad}(\Psi_i)\boldsymbol{U}.\overrightarrow{grad}(\Psi_j)d\Omega$$

U is a vector with the components U, V and W.
FORMUL = 'MATVGR '
(subroutines with names which start with `MT05`)
Matrix used for the convection term with centred discretisation.

$$N(i,j) = XMUL\int_\Omega \Psi_i\boldsymbol{U}.\overrightarrow{grad}(\Psi_j)d\Omega$$

U is a vector with the components U, V and W.
FORMUL = 'FMATMA '

(subroutines with names which start with `MT06`)
Matrix used for conservative smoothing.

$$N(i,j) = XMUL \int_{\Omega} F\Psi_i\Psi_j d\Omega$$

<u>FORMUL = 'MSLUMP '</u>
(subroutines with names which start with `MT07`)
Mass matrix with local mass-lumping.

$$N(i,j) = XMUL \int_{\Omega} (1-F)\Psi_i + F\Psi_i\Psi_j d\Omega$$

Here, F must be a P0 function, that is, constant for each element. If the value of F is locally 0, the mass-matrix will be locally lumped into a diagonal.
<u>FORMUL = 'MATFGR X'</u>
(subroutines with names which start with `MT08`)
$N(i,j) = -XMUL \int_{\Omega} \Psi_j F \frac{\partial \Psi_i}{\partial x} d\Omega$
Beware the minus sign !!!!!!
If FORMUL(16:16) is equal to 'Y' or 'Z' instead of 'X', the derivative will be obtained according to y or z.
<u>FORMUL = 'MATQGR '</u>
(subroutines with names which start with `MT09`)

$$N(i,j) = XMUL \int_{\Omega} \Psi_i F \boldsymbol{U}.\overrightarrow{grad}(\Psi_j) d\Omega$$

Subroutines with names which start with `MT10` are not yet programmed.
<u>FORMUL = 'MATGRF X'</u>
(subroutines with names which start with `MT11`)
$N(i,j) = -XMUL \int_{\Omega} \Psi_j \frac{\partial (F\Psi_i)}{\partial x} d\Omega$
Beware the minus sign !!!!
If FORMUL(16:16) is equal to 'Y' or 'Z' instead of 'X', the derivatives will be obtained according to y or z.
<u>FORMUL = 'MATUGH X'</u>
(subroutines with names which start with `MT12`)
Matrix used for the method SUPG, options 1 and 2.

$$N(i,j) = XMUL \int_{\Omega} \Psi_j \frac{\partial F}{\partial x} \boldsymbol{U}.\overrightarrow{grad}(\Psi_i) d\Omega$$

If FORMUL(16:16) is equal to 'Y' or 'Z' instead of 'X', the derivatives will be obtained according to y or z.
$\boldsymbol{U}$ is a vector with the components U, V and W.
<u>FORMUL = 'MATGRA X'</u>
(subroutines with names which start with `MT13`)
Gradient matrix.

$$N(i,j) = XMUL \int_{\Omega} \frac{\partial \Psi_j}{\partial x} \Psi_i d\Omega$$

If FORMUL(16:16) is equal to 'Y' or 'Z' instead of 'X', the derivatives will be obtained according to y or z.
<u>FORMUL = 'MAMURD PSI'</u> or <u>FORMUL = 'MAMURD2 PSI'</u>
(subroutines with names which start with `MT14`)

Distribution matrix in case of use of the Multidimensional Upwind Residual Distribution scheme in 3D. See reference J.-M. et al. [4] for more details.
If FORMUL(14:16) is equal to ' N' instead of 'PSI' the matrix will be assembled.
FORMUL = 'FFBT '
(subroutines with names which start with `MT99`)
This is in fact a series of different matrices and the string FORMUL(8:16) is also used for defining the formula. For example if FORMUL(8:16)=' 0XX0', the matrix will be:

$$N(i,j) = XMUL \int_{\Omega} F \frac{\partial F}{\partial x} \frac{\partial \Psi_j}{\partial x} \Psi_i d\Omega$$

Explanation: the term in the integral is a product of 4 terms based, for the first 2, on the vector F, and then on the Basis function called here B and the test function called T.
If the first character is 0, the first term will be F. If the first character is X, the first term will be $\frac{\partial F}{\partial x}$. If the first character is Y, the first term will be $\frac{\partial F}{\partial y}$.
Then we proceed to second character and again function F, to third character and function Ψ_j, to fourth character and function Ψ_i.
Up to now the combinations 0XX0, 0YY0, XX00, 0X0Y, XY00, YY00, 0Y0X are implemented. The formula FORMUL(8:16)='00XX+00YY' is also available. Note that missing combinations can be obtained because the first two characters can be exchanged. Moreover exchanging the last two characters gives the transposed matrix of the previous formula.
The existing subroutines building matrices in version 6.2 are the following, their function can be deduced from the explanations above:

mt01aa.f	mt01bb.f	mt01cc.f	mt01oo.f	mt01pp.f
mt01tt.f	mt02aa.f	mt02aa_2.f	mt02bb.f	mt02cc.f
mt02pp.f	mt02pt.f	mt02tt.f	mt03aa.f	mt03bb.f
mt03cc.f	mt04aa.f	mt04bb.f	mt04cc.f	mt04pp.f
mt04tt.f	mt05aa.f	mt05bb.f	mt05cc.f	mt05pp.f
mt05tt.f	mt06aa.f	mt06bb.f	mt06cc.f	mt06ff.f
mt06ft.f	mt06ft2.f	mt06oo.f	mt06oc.f	mt06pp.f
mt06tt.f	mt07aa.f	mt07bb.f	mt07cc.f	mt08aa.f
mt08ab.f	mt08ac.f	mt08ba.f	mt08bb.f	mt08pp.f
mt08tt.f	mt11aa.f	mt11ab.f	mt11ac.f	mt11ba.f
mt11bb.f	mt12aa.f	mt12ab.f	mt12ac.f	mt12ba.f
mt12bb.f	mt13aa.f	mt13ab.f	mt13ba.f	mt13bb.f
mt13cc.f	mt13ca.f	mt14pp.f	mt99aa.f	

4.3.2 Construction of vectors

```
SUBROUTINE VECTOR( VEC,OP,FORMUL,IELM1,
   XMUL,F,G,H,U,V,W,
   MESH,MSK,MASKEL )
```

The principle is the same as for MATRIX. The result is the vector VEC, with discretisation IELM1, constructed according to FORMUL and the operation OP (see below).
XMUL, F ,G ,H ,U ,V ,W are respectively a constant and six vector structures used in the definition of the new vector. The discretisation of F, G, H, U, V and W is checked and is taken into account for the calculations.
the other arguments are the same as for MATRIX:
Possible operations
OP may be equal to :

- '=' : in this case the vector corresponds to the formula indicated.
- '+' : the formula indicated is added to VEC.

Available formulae

FORMUL is a string of 16 characters the first 6 of which take the name of the equivalent former subroutine in BIEF version 3.0 (for certain, however, the meaning has been changed). The sixteenth character is sometimes used to specify the derivatives and may then contain the characters X, Y or Z.
All the possible formulae are given below. However, all the discretisation combinations are not programmed. If a vector has not been programmed, an error message will appear to this effect.
In the next part of the text, Ψ_i is the base corresponding to the element IELM1. The example of dimension 3 is given. For the other dimensions, some terms would of course have to be removed. The names of the corresponding subroutines in BIEF 3.2 are given in brackets.
FORMUL = 'MASBAS '
(subroutines with names which start with `VC00`)
Integrals of the bases, or product of a mass matrix by a vector with the value of 1 everywhere.

$$VEC(i) = XMUL \int_\Omega \Psi_i d\Omega$$

FORMUL = 'MASVEC '
(subroutines with names which start with `VC01`)
Product of a mass matrix by a vector F.

$$VEC(i) = XMUL \int_\Omega F\Psi_i d\Omega$$

FORMUL = 'SUPG '
(subroutines with names which start with `VC03`)

$$VEC(i) = XMUL \int_\Omega \boldsymbol{K}\overrightarrow{grad}(\Psi_i)\boldsymbol{U}\overrightarrow{grad}(F) d\Omega$$

$\boldsymbol{U}$ is a vector with the components U, V and W.
$\boldsymbol{K}$ is a vector with the components G and H. (this would have to be modified in dimension 3).
FORMUL = 'VGRADP ' or 'VGRADP2 ' (used in 3D only)
(subroutines with names which start with `VC04`)

$$VEC(i) = XMUL \int_\Omega \boldsymbol{U}_{2D}\overrightarrow{grad}_{2D}(\Psi_i) d\Omega$$

$\boldsymbol{U}$ is a vector with the components U and V.
VGRADP is the same formula, with corrections when the generalised sigma transformation is used.
FORMUL = 'FLUBOR '
(subroutines with names which start with `VC05`)

$$VEC(i) = XMUL \int_\Gamma \Psi_i \boldsymbol{U}\boldsymbol{n} d\Gamma$$

$\boldsymbol{U}$ is a vector with the components U, V and W.
$\boldsymbol{n}$ is the normal outer vector.
FORMUL = 'FLUBOR2 '
In 3D only, FLUBOR2 is like FLUBOR, but in the case of a generalised sigma transformation.
FORMUL = 'VGRADF '

(subroutines with names which start with `VC08`)

$$VEC(i) = XMUL \int_{\Omega} \Psi_i \boldsymbol{U} \overrightarrow{grad}(F) d\Omega$$

U is a vector with the components U, V and W.
FORMUL = 'QGRADF '
(subroutines with names which start with `VC09`)

$$VEC(i) = XMUL \int_{\Omega} \Psi_i G \boldsymbol{U} \overrightarrow{grad}(F) d\Omega$$

U is a vector with the components U, V and W.
FORMUL = 'FLUBDF '
(subroutines with names which start with `VC10`)

$$VEC(i) = XMUL \int_{\Gamma} \Psi_i F \boldsymbol{U} \boldsymbol{n} d\Gamma$$

U is a vector with the components U, V and W. ***n*** is the normal vector external to the domain.
FORMUL = 'GGRADF X'
(subroutines with names which start with `VC11`)

$$VEC(i) = XMUL \int_{\Omega} \Psi_i G \overrightarrow{grad}(F) d\Omega$$

If FORMUL(16:16) is equal to 'Y' or 'Z' instead of 'X', the derivative will be obtained according to y or z.
FORMUL = 'GRADF X'
(subroutines with names which start with `VC13`)

$$VEC(i) = XMUL \int_{\Omega} \Psi_i \overrightarrow{grad}(F) d\Omega$$

If FORMUL(16:16) is equal to 'Y' or 'Z' instead of 'X', the derivative will be obtained according to y or z.
In 3 dimensions, variants are available:

- GRADF(X,Y) X and GRADF(X,Y) Y will consider only the gradient of a function which does not depend on Z.
- GRADF2 will take care of hydrostatic inconsistencies.

FORMUL = 'PRODF '
(subroutines with names which start with `VC14`)

$$VEC(i) = XMUL \int_{\Omega} \Psi_i F (2(\frac{\partial U}{\partial x})^2 + 2(\frac{\partial V}{\partial y})^2 + (\frac{\partial U}{\partial y} + \frac{\partial V}{\partial x})^2) d\Omega$$

This vector is used in the calculation of the turbulent production with the model k-epsilon.
FORMUL = 'DIVQ '
(subroutines with names which start with `VC15`)

$$VEC(i) = XMUL \int_{\Omega} \Psi_i div(F\boldsymbol{U}) d\Omega$$

U is a vector with the components U, V and W.
FORMUL = 'SUPGDIVU '
(subroutines with names which start with `VC16`)

$$VEC(i) = XMUL \int_{\Omega} \boldsymbol{K} grad(\Psi_i) div(\boldsymbol{U}) d\Omega$$

$\boldsymbol{U}$ is a vector with the components U, V and W. $\boldsymbol{K}$ is a vector with the components F, G and H.
FORMUL = 'FLUDIF '
(subroutines with names which start with `VC17`)

$$VEC(i) = XMUL \int_{\Omega} \Psi_i U.\overrightarrow{grad}(F).\boldsymbol{n} d\Omega$$

This is not currently used nor implemented.
FORMUL = 'VGRADF2 '
(subroutines with names which start with `VC18`)

$$VEC(i) = XMUL \int_{\Omega} \Psi_i U.\overrightarrow{grad}(F) d\Omega$$

This is specifically for 3D computations with prisms, and unlike VGRADF, the test function Ψ_i is here a 2-dimensional test function (no dependency on z). This is used by TELEMAC-3D in subroutine WSTARW.
FORMUL = 'HUGRADP '
(subroutines with names which start with `VC19`)

$$VEC(i) = XMUL \int_{\Omega} F\boldsymbol{U}.\overrightarrow{grad}(\Psi_i) d\Omega$$

This is used in 2D, mostly for computing fluxes. H in HUGRADP stands for the depth denoted h, which can be misleading as it does not refer to the function H which is an argument of subroutine VC19AA. A variant HUGRADP2 exists, in this case the velocity is not only $\boldsymbol{U}$ of components (U,V), but $\boldsymbol{U} + G\overrightarrow{grad}(H)$. This is a way of treating the gradient of the free surface elevation as a piecewise constant function, which it is in reality when the depth is linear.
The existing subroutines building vectors in version 6.2 are the following, their function can be deduced from the explanations above:

vc00aa.f	vc00bb.f	vc00cc.f	vc00pp.f	vc00pp2.f
vc00ft.f	vc00ff.f	vc00tt.f	vc01aa.f	vc01bb.f
vc01ff.f	vc01ft.f	vc01oo.f	vc01pp.f	vc01tt.f
vc01tt0.f	vc03aa.f	vc03bb.f	vc04aa.f	vc04pp.f
vc05oo.f	vc05aa.f	vc04tt.f	vc05ff.f	vc05ft.f
vc08aa.f	vc08bb.f	vc08cc.f	vc08pp.f	vc08tt.f
vc09aa.f	vc10oo.f	vc11aa.f	vc11aa2.f	vc11bb.f
vc11pp.f	vc11tt.f	vc11tt0.f	vc13aa.f	vc13bb.f
vc13cc.f	vc13pp.f	vc13pp2.f	vc13tt.f	vc14aa.f
vc15aa.f	vc16aa.f	vc18pp.f	vc19aa.f	

4.4 Operations on matrices and vectors

Some operations described below also apply to vectors contained in blocks, since it is possible to place these blocks in the subroutine arguments.

4.4.1 Operations on vectors

syntax:

```
SUBROUTINE OS(OP,X,Y,Z,C,[IOPT,INFINI,ZERO])
```

Arguments:

OP is a string of 8 characters describing an operation between X,Y,Z and C.

X is a vector or a working array which will contain the result of the operation.

Y and Z are vector structures. Y and Z can be dummy arguments if they do not appear in the operation, but they must be declared as BIEF_OBJ structures. C is a double precision real number.

X,Y,Z,C,IOPT, INFINI and ZERO are optional, the last 3 are used only when a division is implied in the operation asked, for example if OP = 'X=Y/Z '. When they are present, it is better to name them as is done in the following line:

```
CALL OS('X=Y/Z   ',U,V,W,0.D0,IOPT=2,INFINI=1.D0,ZERO=1.D-10)
```

If IOPT = 1 : no check of division by 0 is made.
If IOPT = 2 : the infinite terms are replaced by the constant INFINI.
If IOPT = 3 : stop in the case of division by a number less than the parameter ZERO.
If IOPT = 4 : infinite terms are truncated at the value 1.D0/ZERO or -1.D0/ZERO (depending on their sign).

Warning:
The structure of X is updated according to the result. Consistency checks between X, Y and Z are applied. Y and Z must have the same discretisation.

Very important note:
When Y is mentioned in the operation and X and Y have different characteristics, the conflict is settled by copying the characteristics of Y onto those of X (by a call to CPSTVC). This is done without any warning message and means that vectors can be used as working arrays. Only vectors allocated with a status equal to 1 will trigger an error message if a change of their discretisation is tried.
The operation OP may be :

- OP = 'X=C ' : C VALUE ASSIGNED TO ALL COMPONENTS OF X
- OP = 'X=0 ' : C VALUE ASSIGNED TO ALL COMPONENTS OF X
- OP = 'X=Y ' : Y COPIED ON TO X
- OP = 'X=+Y ' : IDEM
- OP = 'X=-Y ' : -Y COPIED ON TO X
- OP = 'X=1/Y ' : INVERSE OF Y COPIED ON TO X
- OP = 'X=Y+Z ' : SUM OF Y AND Z COPIED ON TO X
- OP = 'X=Y-Z ' : DIFFERENCE OF Y AND Z COPIED ON TO X
- OP = 'X=YZ ' : PRODUCT Y BY Z COPIED ON TO X

- OP = 'X=-YZ ' : PRODUCT Y BY Z COPIED ON TO X
- OP = 'X=XY ' : PRODUCT Y BY X COPIED ON TO X
- OP = 'X=X+YZ ' : PRODUCT Y BY Z ADDED TO X
- OP = 'X=X-YZ ' : PRODUCT Y BY Z SUBSTRACTED FROM X
- OP = 'X=CXY ' : PRODUCT OF C X AND Y COPIED ON TO X
- OP = 'X=CYZ ' : PRODUCT OF C, Y AND Z COPIED ON TO X
- OP = 'X=CXYZ ' : PRODUCT OF C, X, Y AND Z COPIED ON TO X
- OP = 'X=X+CYZ ' : PRODUCT OF C, Y AND Z ADDED TO X
- OP = 'X=Y/Z ' : DIVISION OF Y BY Z COPIED ON TO X
- OP = 'X=CY/Z ' : PRODUCT OF C BY Y DIVIDED BY Z ET COPIED ONTO X
- OP = 'X=CXY/Z ' : PRODUCT C X Y DIVIDED BY Z AND COPIED ON X
- OP = 'X=X+CY/Z' : PRODUCT OF C BY Y DIVIDED BY Z ADDED TO X
- OP = 'X=X+Y ' : Y ADDED TO X
- OP = 'X=X-Y ' : Y SUBSTRACTED FROM X
- OP = 'X=CX ' : X MULTIPLIED BY C
- OP = 'X=CY ' : CY COPIED ON TO X
- OP = 'X=Y+CZ ' : CZ ADDED TO Y AND COPIED ON TO X
- OP = 'X=X+CY ' : CY ADDED TO X
- OP = 'X=SQR(Y)' : SQUARE ROOT OF Y COPIED ON TO X
- OP = 'X=ABS(Y)' : ABSOLUTE VALUE OF Y COPIED ON TO X
- OP = 'X=N(Y,Z)' : X NORM OF THE VECTOR WITH COMPONENTS Y,Z
- OP = 'X=Y+C ' : C ADDED TO Y COPIED ON TO X
- OP = 'X=X+C ' : C ADDED TO X
- OP = 'X=Y**C ' : Y AT THE POWER OF C COPIED ON TO X
- OP = 'X=COS(Y)' : COSINE OF Y COPIED ON TO X
- OP = 'X=SIN(Y)' : SINE OF Y COPIED ON TO X
- OP = 'X=ATN(Y)' : ARCTG OF Y COPIED ON TO X
- OP = 'X=A(Y,Z)' : INVERSE OF TANGENT Y/Z COPIED ON TO X
- OP = 'X=+(Y,C)' : X = MAX OF Y AND C
- OP = 'X=-(Y,C)' : X = MIN OF Y AND C

- OP = 'X=+(Y,Z)' : X = MAX OF Y AND Z
- OP = 'X=-(Y,Z)' : X = MIN OF Y AND Z
- OP = 'X=YIFZ<C' : FOR EACH POINT : X = Y IF Z < C
- OP = 'X=C(Y-Z)' : X = C*(Y-Z)

Examples:

```
CALL OS('X=0     ',X=TAB)
```

will set the double precision array of BIEF_OBJ structure TAB to zero.

```
CALL OS('X=Y+Z   ',X=TRAV1,Y=U,Z=V)
```

will copy the sum of U and V on to TRAV1.

```
CALL OS('X=Y+Z   ',TRAV1,U,V)
```

will have the same effect. As all the arguments are present up to Z, there is no ambiguity.
syntax:

```
SUBROUTINE OV(OP,X,Y,Z,C,NPOIN)
```

OV carries out the same operations as OS (it is called by OS), but directly on double precision arrays and without consistency checks or structure updating. The argument NPOIN indicates the number of values on which the operation must be conducted.
syntax:

```
SUBROUTINE OV_2(OP,X,IX,Y,IY,Z,IZ,C,NPOIN)
```

`OV_2` carries out the same operations as OV, but it is possible to choose the vector dimension concerned by the operation. These dimension numbers are indicated by IX, IY and IZ.
The instruction:

```
CALL OV_2(OP,X,2,Y,5,Z,3,C,NPOIN)
```

thus replaces the former instruction:

```
CALL OV(OP,X(1,2),Y(1,5),Z(1,3),C,NPOIN)
```

where X, Y and Z were declared as two-dimensional arrays.
syntax:

```
SUBROUTINE OVD(OP,X,Y,Z,C,IOPT,INFINI,ZERO,NPOIN)
```

`OVD` carries out the same operations as OS (it is called by OS), but directly on double precision arrays and without consistency checks or structure updating. The argument NPOIN indicates the number of values on which the operation must be conducted.
syntax:

```
SUBROUTINE OVD_2(OP,X,DIMX,Y,DIMY,Z,DIMZ,C,DIM1,NPOIN,IOPT,INFINI,ZERO)
```

`OVD_2` is comparable to OVD but acts on 2-dimensional vectors, the second size being DIM1. `OVD_2` will actually call `OVD` with X(1,DIMX), Y(1,DIMY) and Z(1,DIMZ) as arguments instead of X, Y and Z.

DIM1 is the first dimension of vectors X, Y and Z.

syntax:

```
SUBROUTINE OSBD(OP,X,Y,Z,C,MESH)}
```

The form and the principle are the same as for OS but the array MESH (mesh structure) is given as a last argument. In this case we have vectors which would be refused by OS because of lack of consistency. For `OSBD`, X is defined on the boundaries and Y and Z are vectors defined on the whole domain. There is thus data retrieval of Y and Z, which requires the presence of MESH.
The possible operations are as follows:

- OP = 'X=Y ': BOUNDARY VALUES OF Y COPIED ON TO X
- OP = 'X=+Y ': IDEM
- OP = 'X=X+Y ': BOUNDARY VALUES OF Y ADDED TO X
- OP = 'X=Y+Z ': BOUNDARY VALUES OF Y AND Z ADDED TO X
- OP = 'X=X-Y ': BOUNDARY VALUES OF Y SUBSTRACTED TO X
- OP = 'X=CY ': BOUNDARY VALUES OF CY COPIED ON TO X
- OP = 'X=X+CY ': BOUNDARY VALUES OF CY ADDED TO X
- OP = 'X=CXY ': BOUNDARY VALUES OF CXY COPIED ON TO X

All the arguments are mandatory.
syntax:

```
SUBROUTINE OVBD(OP,X,Y,Z,C,NBOR,NPTFR)
```

Same role as `OSBD` but by giving the general numbering of the boundary points and the number of boundary points. `OVBD` does not conduct any check.
syntax:

```
SUBROUTINE OSDB(OP,X,Y,Z,C,MESH)
```

Same principle as for `OSBD`. Here, X is defined on the entire domain and Y and Z are vectors defined on the boundaries. Only the X values corresponding to boundary points are filled.
The following operations are possible:

- OP = 'X=Y ' : Y COPIED ON TO X
- OP = 'X=+Y ' : IDEM
- OP = 'X=X+Y ' : Y ADDED TO X
- OP = 'X=X-Y ' : Y SUBSTRACTED FROM X
- OP = 'X=CY ' : CY COPIED ON TO X
- OP = 'X=Y+Z ' : Y+Z COPIED ON TO X
- OP = 'X=X-YZ ' : YZ SUBSTRACTED FROM X
- OP = 'X=X+CY ' : CY ADDED TO X
- OP = 'X=XY ' : X MULTIPLIED BY Y

syntax:

```
SUBROUTINE OSDBIF(OP,X,Y,Z,C,INDIC,CRITER,MESH)
```

Same principle as for `OSDB` but a test is done. If INDIC(K)=CRITER, the operation OP is done on index number K of vector X.
The following operations are possible:

- OP = 'X=Y ' : Y COPIED ON TO X
- OP = 'X=+Y ' : IDEM

INDIC is an integer array (not a structure).

CRITER is a given integer.

syntax:

```
SUBROUTINE OVDB(OP,X,Y,Z,C,NBOR,NPTFR)
```

Same role as `OSDB` but by giving data from MESH, the general numbering of the boundary points and the number of boundary points. OVDB does not conduct any check.

4.4.2 Operations on matrices

syntax:

```
SUBROUTINE OM(OP,M,N,D,C,MESH)
```

`OP` is the operation to be carried out. M and N are two matrices, D a diagonal and C a constant. N, D and C are only used when they are part of the operation. MESH is the integer block of the mesh.
The following operations are possible:

- OP = 'M=N ' : COPY OF N ON TO M
- OP = 'M=TN ' : COPY OF TRANSPOSED OF N ON TO M
- OP = 'M=CN ' : PRODUCT OF N BY THE C CONSTANT
- OP = 'M=M+CN ' : CN ADDED TO M
- OP = 'M=M+CTN ' : C TIMES TRANSPOSED OF N ADDED TO M
- OP = 'M=M+N ' : N ADDED TO M
- OP = 'M=M+TN ' : TRANSPOSED OF N ADDED TO M
- OP = 'M=MD ' : RIGHT HAND PRODUCT OF M BY D
- OP = 'M=DM ' : LEFT HAND PRODUCT OF M BY D
- OP = 'M=DMD ' : LEFT AND RIGHT HAND PRODUCT OF M BY D
- OP = 'M=0 ' : M COMPONENTS ARE SET TO 0
- OP = 'M=X(M) ' : CHANGE TO A NON SYMMETRICAL FORM
- OP = 'M=MSK(M)' : MASKING EXTRADIAGONAL TERMS
- OP = 'M=M-DN ' : REMOVING DN FROM M
- OP = 'M=M-ND ' : REMOVING ND FROM M

- OP = 'M=M+D ' : Diagonal D added to M

When the operation only concerns M, it is advisable to repeat M instead of the argument N. In all cases N should be a matrix-structure, or it may generate inexplicable crashes.
It is possible that a few of these operations are not yet programmed with all the matrix-storage.
syntax:

```
SUBROUTINE LUMP(DIAG,A,MESH,XMUL)
```

Returns a vector representing a diagonal matrix DIAG (in fact a `BIEF_OBJ` structure with a vector type) containing the sum of the rows of the matrix A. The other arguments are given below:

MESH esh structure.

XMUL Multiplying factor.

4.4.3 Matrix x vector products

syntax:

```
SUBROUTINE MATVEC(OP,X,A,Y,C,MESH,[LEGO])
```

The result is the vector X (BIEF_OBJ structure) which, depending on the operation OP, contains different combinations of X, C and the product of A and Y:

- OP = 'X=AY ' : X = AY
- OP = 'X=X+AY ' : X = X + AY
- OP = 'X=X-AY ' : X = X - AY
- OP = 'X=X+CAY ' : X = X + C AY
- OP = 'X=TAY ' : X = TA Y (TRANSPOSED OF A)
- OP = 'X=X+TAY ' : X = X + TA Y
- OP = 'X=X-TAY ' : X = X - TA Y
- OP = 'X=X+CTAY' : X = X + C TA Y

The other arguments are:

MESH Mesh integer structure.

Optional argument:

LEGO Logical.

If LEGO is equal to .FALSE., the vector X will not be assembled and part of the result (due to the off-diagonal terms of A) will be contained in the array W of structure MESH. The vector X will contain only the contribution of the diagonal.
The aim of LEGO=.FALSE. is to save on assemblies during calculations where X is the sum of several matrix x vector products.
Thus to calculate X = A Y + B Z, the following two calls will be made one after the other:

```
CALL MATVEC('X=AY    ',X,A,Y,C,MESH,LEGO=.FALSE.)
CALL MATVEC('X=X+AY  ',X,B,Z,C,MESH,LEGO=.TRUE.)
```

This will save on the assembly of the product A Y.
syntax:

```
SUBROUTINE MATRBL(OP,X,A,Y,C,MESH)
```

The principle is the same as MATVEC but MATRBL applies to blocks.
If A is a block of 4 matrices. X and Y must be blocks of 2 vectors.
If A is a block of 9 matrices. X and Y must be blocks of 3 vectors.
The only operations that are possible for the moment are:

- OP = 'X=AY ' : X = AY
- OP = 'X=TAY ' : X = TA Y (TRANSPOSED OF A)

4.5 Solving linear systems

The processing of a linear system is handled entirely by the subroutine SOLVE, except for the Dirichlet-type boundary conditions processed by DIRICH (see also 5.3.5).
syntax:

```
SUBROUTINE DIRICH( F,S,SM,FBOR,LIMDIR,WORK,MESH,KDIR,MSK,MASKPT)
```

F Initial and future solution of the system

S System matrix

SM Right hand side of system ("Second membre" in French)

FBOR Dirichlet point boundary condition

LIMDIR Boundary conditions type if LIMDIR(K) = KDIR the K^{th} boundary point is a Dirichlet type point.

WORK Working array block.

KDIR Convention for Dirichlet conditions

MESH BIEF_MESH structure

MSK if YES, presence of masked elements

MASKPT Masked points array

- =1 : Normal
- =0 : Masked point

If S is a block of 4 or 9 matrices, F must be a block of 2 or 3 vectors, LIMDIR must be an array with 2 or 3 dimensions, and FBOR must be an array of 2 or 3 vectors.
DIRICH will modify the matrices and right hand sides of the system to take into account the prescribed values.
syntax:

```
SUBROUTINE SOLVE(X,A,B,TB,CFG,INFOGR,MESH,AUX)
```

X Solution vector.

A System matrix.

B Second member of system.

TB Block containing working arrays.

CFG Solver configuration.

INFOGR if .TRUE., information will be printed.

MESH BIEF_MESH structure.

AUX Matrix used for preconditioning. Not used by diagonal preconditioning

Here is the meaning of options stored in the SLVCFG structure called above CFG:

CFG%SLV **1** Conjugate gradient
- **2** Conjuguate residual
- **3** Normal equation on conjugate gradient
- **4** Minimal error
- **5** Conjugate gradient squared
- **6** Conjugate gradient squared stabilised
- **7** Gmres

CFG%KRYLOV Only used by GMRES. The option is the dimension of Krylov's space (see ref. J.-M. [2]).

CFG%PRECON Preconditioning choice.

- **1** Nothing
- **2** Diagonal preconditioning
- **3** Block-diagonal preconditioning
- **5** Diagonal preconditioning with absolute values of diagonal
- **7** Crout preconditioning
- **11** Gauss-seidel ebe preconditioning
- **13** Matrix given by the user
- **17** Specific to TELEMAC-3D. Direct solution on verticals are used as preconditioning.

CFG%EPS Relative accuracy requested, or absolute if norm of the right-hand side is less than 1..

CFG%ZERO Epsilon for the divisions by zero.

CFG%NITMAX Maximum number of iterations.

TB will be used by `SOLVE` to find `BIEF_OBJ` structures with working arrays. The number of structures to be placed in TB depends on the method chosen. At the time being, the minimum number of arrays in TB must be:
`S*MAX(7,2+2*METHOD%KRYLOV)` where S is 1 if the system is made of 1 matrix, 2 for blocks of 4 matrices (2 unknowns like in ARTEMIS) and 3 for blocks of 9 matrices (3 unknowns like in TELEMAC-2D).

4.6 Parallelism

Parallelism consists of using simultaneously a cluster of computers, or a group of processors in the same computer, to solve a single problem. Using n processors would ideally divide by n the time necessary to solve the same problem with only one processor. The task would be easy if the problem could be broken down into sub-tasks, independent of each other. It becomes much more difficult when each processor needs the results from the others. We will focus hereafter on parallelism performed with processors having each its own memory, and communicating with the others via message transmission, this is the case with networks of work stations or PC's and is known as distributed-memory parallelism.
Many experiments in automatic parallelism, where compilers themselves perform the task of optimizing the program, showed very poor improvement in CPU time. Furthermore, vectorization and parallelism appeared to be contradictory. Vectorization requires simple loops to perform sub-tasks whereas distributed-memory parallelism hands over complex tasks to each processor so as to optimize communication time and data transmission time. Efficiently vectorized software would be naturally poorly parallelized. As an example, the assembly loops resulting from an EBE matrix-vector product cannot be accelerated by more than a ratio of two even if we overlook the communication time. This is due to the fact that the results of each processor have to be assembled. That leads to a new cost which limits drastically the overall time to be gained. This is known as a granularity problem, the size of the tasks to be parallelized being too small. It is unlikely that progress in the algorithm would help in solving this theoretical bottleneck. From that, the idea emerges to break up the problem in another way: not by isolating small tasks but in a kind of geographical way, by decomposing the domain of computation. This idea of domain decomposition aims at assigning onto each processor one part of the domain over which it would solve the fluid mechanics problem. The implementation is quite easy in the case of explicit algorithms: each equation is only a function of the variables related to the nodes in the immediate vicinity, computed at the earlier time step. Each processor is then in charge of the equations related to a group of nodes, and of the data concerning the neighbours of these nodes, resulting from the previous time step. This is executed merely by a partition of the domain, with an overlap of one element, and data transmission at the end of each time step. In the case of our implicit algorithms, and especially with linear systems solved on the whole domain, the implementation is more complex, though possible. In fact, we can guarantee that the results of a parallel computation will be the same as a scalar computation, except for truncation errors because computations will not be performed in the same order. Parallelism (initially implemented on our algorithms by Reinhard Hinkelmann at the University of Hanover can be limited to the following problems:

- Partition of the domain,
- Communication between processors.
- Implementation of some basic algorithms: vector assembly, dot product, computation of normal vector and so on.

We will examine these three points hereafter.

4.6.1 Partition of the domain

In the case of finite element meshes and implicit algorithms, it is better to partition without overlapping, edge to edge. The specifications for an efficient domain decomposer would be the following:

- realizing a partition of meshes of triangles (the sub-domains of three-dimensional meshes of prisms will be made from sub-domains of triangles).

- partitioning the domain into blocks in order to ensure a balance between the processors. Because the main algorithms are made of loops over the elements and nodes, the partition will guarantee a balance between the numbers of elements, or similarly between the number of nodes within each sub-domain.
- minimizing the number of nodes shared by different sub-domains and for which communications between processors will be necessary.

We currently use the Metis mesh partitioner, which is available on the web site: `http://www-users.cs.umm.edu/~karypis/metis`.

4.6.2 Data structure specific to parallelism

We describe here some of the data structures that will be often used in parallelism.
Each sub-domain is assigned to a processor together with the information of a standard domain (connectivity table IKLE, nodes coordinates and so on) but also with additional information, to help in assembling the results over the whole domain at the end of the computation. This information is as follows:

- an array KNOLG storing the global numbers of the nodes in the whole mesh. The inverse array, KNOGL, is defined within a loop:

```
DO I=1,NPOIN
  KNOGL(KNOLG(I))=I
ENDDO
```

- an array NACHB whose dimension is (5,NPTIR), where NPTIR is the number of the interfacial nodes between the sub-domain and the others. These interfacial nodes are numbered from 1 to NPTIR. NACHB(1,IR) is the global number of the interfacial node IR. This array gathers the information to be transmitted to the others processors. The integers NACHB(2,IR) to NACHB(5,IR) are the numbers of the other sub-domains which the nodes belong to. They may have a -1 value if these sub-domains are less than 4. The dimension 5 must be increased if a node belongs to more than 5 sub-domains.

Some additional information has to be defined on the actual boundary nodes of a 2-dimensional domain:

- ISEG, XSEG, YSEG and NUMLIQ.
  - If ISEG >0: the boundary node just after belongs to another sub-domain, its global number is ISEG, and its real coordinates are XSEG and YSEG.
  - If ISEG <0: the boundary node just before belongs to another sub-domain, its global number is -ISEG, and its real coordinates are XSEG and YSEG.
  - If ISEG = -999999: the node verifies the two conditions above (this pathological case is not considered by the software).

  The latest algorithms designed in Telemac replaced the use of XSEG and YSEG by parallel communications, thus these arrays could be removed in a near future.

- the integer array NUMLIQ is a specific numbering of the liquid boundaries, which allows association of boundary conditions to them, e.g. an imposed discharge. A numbering is easy to define when the whole domain is known. A possible convention is to start the numbering of these liquid boundaries (inflow and outflow) from the extreme south-west node of the domain and proceeding in the anti clock-wise way along the edge. In the case of a sub-domain for which it is not possible to go over the whole contour, the numbering must be specified because it cannot be simply recomputed.

- IFAPAR is used by the method of characteristics to compute the paths or trajectories when they cross interfaces between sub-domains. The size is IFAPAR(6,NELEM2), as only 2-dimensional data is required. IFAPAR(1:3,IELEM) gives the processor numbers behind the 3 edges of a triangle. IFAPAR(4:6,IELEM) gives, for the same edges, the local number in its processor of the element behind the edge.

- an array INDPU, inverse of NACHB(1,*) helps storing the data received from the other processors: INDPU(NACHB(1,I))=I. Given the number of an interfacial node, INDPU sends back its global number within the sub-domain.

- an array FAC, providing for each node, the inverse of the number of sub-domains to which it belongs (see the algorithm for dot product hereafter).

4.6.3 Communication between processors

Programming by communicative process requires the use of a library of communication functions, such as PVM or MPI. We currently use MPI version 2. These libraries perform different operations:

- setting up of the parallel machine, that is, organizing the communication between various computers or processors,

- running programs on all the processors (spawn order with PVM). In some cases, one processor has the function of a master, the others being the slaves. The program is first run on the master processor, and includes a start order for the slaves. A group name is given to the computation. Apart from this initialization step, there is then no more hierarchy between the processors.

- various kinds of communication: point to point or collective.

Point to point communication

This is the basic communication between two processors, the receptor and the transmitter. The send function and the receive function can differ depending on the types of data (integers, real numbers, etc.). The functions arguments are:

- identifier of receptor or transmitter,

- address of the data to transmit or receive,

- a message flag.

Transmissions can be made in two ways. Synchronous transmission occurs when waiting for the receptor to be ready; this avoids a copy in the buffer. Asynchronous transmission occurs whatever the state of the reception.

Collective communication

Collective communications use simultaneously all the processors. Three types may be distinguished:

- broadcast: a processor (generally the master) sends the same data to all the slaves,

- synchronization: refers to a barrier which all processors must reach before going on the computation,
- conditional transmission: each processor sends a data and receives in return the sum, the maximum or the minimum of all the data transmitted.

To make the source programs independent of the choice of the communication functions library, it is worth writing an interface library to deal with all the communications between the processors. In Telemac this library is called "parallel". When there is no parallelism involved a fake library "paravoid" is used instead, which does not contain any link to a parallelism library. Only a few functions are necessary:

P_DMAX(X) maximum of X over all the processors. X is a double-precision real.

P_DMIN(X) minimum of X over all the processors. X is a double-precision real.

P_DSUM(X) sum of all the values of X provided by all the processors. X is a double-precision real.

P_IMAX(I) maximum of I over all the processors. I is an integer.

P_IMIN(I) minimum of I over all the processors. I is an integer.

P_ISUM(I) sum of all the values of I provided by all the processors. I is an integer.

P_MAIL(CHAINE,NCAR) broadcasting a character string CHAINE, with a length NCAR, to all the processors.

P_READ(BUFFER,NBYTES,SOURCE,TYPE) reading of NBYTES bytes of data whose type is TYPE, to be stored at the address BUFFER and sent by the processor SOURCE.

P_SYNC stops the processors till all of them call this function.

P_WRIT(BUFFER,NBYTES,DEST,TYPE) writing of NBYTES bytes of data, whose type is TYPE, located at the address BUFFER and intended for the processor DEST.

4.6.4 Adaptation of the algorithms

Dot product

The dot product of two vectors over the whole domain implies local computing first, then summing up over the whole sub-domains. While summing, the interface nodes are taken into account several times. The array FAC is then used to correct this error. The parallel dot product `P_DOT` of the vectors X and Y is written as follows:

```
P_DOT = 0.D0
DO I=1,NPOIN
  P_DOT=P_DOT+X(I)*Y(I)*FAC(I)
ENDDO
P_DOT=P_DSUM(P_DOT)
```

On a vector computer, multiplying by FAC(I) does not affect the time of computation. On the contrary, the call to the `P_SUM` routine causes a synchronization of the processors.

Matrix x vector product

First, building the matrices and computing the product are done locally, independently of the other sub-domains. The result is a vector without any contribution from the neighbour sub-domains, on the interfacial nodes. The missing contributions result from the computation of the vector on the other sub-domains. For example, if the node I belongs to two different sub-domains, for which we get X(I)=3 and X(I)=5 respectively, the actual value of X(I) would be the sum 3+5. This can be achieved if processor 1 sends the value 3 to processor 2 and processor 2 sends the value 5 to processor 1. Although it appears simple, this operation is quite complex to achieve because it can lead to a fatal risk: both processors waiting endlessly for the contribution of the other before sending their own. We describe hereafter the series of operations required, known as "blocking communication". More recently, a non-blocking communication scheme has been implemented by Pascal Vezolles from IBM Europe. Basically this second approach consists of providing MPI with the list of communications to perform, and MPI internal routines will organize the work with their own algorithms.
Communication of data after a matrix-vector product:
Up to version 5.8:
Generally speaking we have a number of processors which much send or receive information to or from the others. The main difficulty is to avoid blocked situations where two processors would wait to receive information from each other before sending their own, hence the definition of higher rank and lower rank processors. We have kept the explanations on this obsolete implementation because it really tackles the problem, while the new implementation from version 5.9 on only uses the capabilities of the MPI language, namely the non blocking communication with subroutines `MPI_IRECV` and `MPI_ISEND`.
The transmission is split into 4 different tasks, depending on the rank of the processors:

- transmission of the data to the higher rank processors.
- reception by the higher rank processors.
- transmission of the data to the lower rank processors.
- reception by the lower rank processors.

New data are required for every processor. Each processor prepares its own numbering of higher rank and lower rank processors as well as a numbering of nodes interfacing with each of these processors. 4 new arrays IKP, NHP, IKM and NHM are necessary to navigate from one numbering to another:

- IKP(NBMAXDSHARE,2): IKP(IZH,1) refers to the processor which is the IZH^{th} local higher rank processor. IKP(IZH,2) is the number of interfacial nodes shared with this processor. NBMAXDSHARE is defined in BIEF_DEF where it is set to 80. It is the maximum number of sub-domains neighbouring a given sub-domain.
- IKM(NBMAXDSHARE,2): IKM(IZH,1) refers to the processor which is the IZH^{th} local lower rank processor. IKM(IZH,2) is the number of interfacial nodes shared with this processor.
- NHP(NBMAXDSHARE,NPTIR): NHP(IZH,IR) is the global number in the sub-domain of a point whose number is IR in the interface with theIZH^{th} higher rank processor.
- NHM(NBMAXDSHARE,NPTIR): NHM(IZH,IR) is the global number in the sub-domain of a point whose number is IR in the interface with theIZH^{th} lower rank processor.

- ILMAX is the maximum distance in order between the processor and its neighbours. It will restrict the size of the loops over these neighbours.

Considering this information, the data transmission for vector V (defined over the whole domain) and for processor IPID, is written as follows:

1. storage of the data to be sent in a first buffer

```
DO I=1,NPTIR
  BUF(I)=V(NACHB(1,I))
ENDDO
```

2. transmission to higher rank processors, for example processor ILP

   (a) storage of the data relative to the processor in a second buffer

   ```
   DO I=1,IKP(ILP,2)
     ERGBUF(I)=BUF(INDPU(NHP(ILP,I)))
   ENDDO
   ```

   (b) sending

   ```
   CALL P_WRIT(ERGBUF,8*IKP(ILP,2),IKP(ILP,1),
               ABS(IKP(ILP,1)-IPID)
   ```

3. reception from lower rank processors, for example processor ILM

   (a) reception

   ```
   CALL P_READ(ERGBUF,8*IKM(ILM,2),IKM(ILM,1),
               ABS(IKM(ILM,1)-IPID)
   ```

   (b) storage in vector V

   ```
   DO I=1,IKM(ILM,2)
     V(NHM(ILM,I))=V(NHM(ILM,I))+ERGBUF(I)
   ENDDO
   ```

4. transmission to lower rank processors, for example processor ILM

   (a) storage of the data relative to the processor in a second buffer

   ```
   DO I=1,IKM(ILM,2)
     ERGBUF(I)=BUF(INDPU(NHM(ILM,I)))
   ENDDO
   ```

   (b) sending

   ```
   CALL P_WRIT(ERGBUF,8*IKM(ILM,2),IKM(ILM,1),
               ABS(IKM(ILM,1)-IPID)
   ```

5. reception from upper rank processors, for example processor ILP

   (a) reception

   ```
   CALL P_READ(ERGBUF,8*IKP(ILP,2), IKP(ILP,1),
               ABS(IKP(ILP,1)-IPID)
   ```

(b) summing into vector V

```
DO I=1,IKP(ILP,2)
  V(NHP(ILP,I))=V(NHP(ILP,I))+ERGBUF(I)
ENDDO
```

This algorithm can be made more complex to process several vectors at the same time or for tasks different from summing.
From version 5.9 on:
The implementation is much easier with the MPI subroutines `MPI_IRECV` and `MPI_ISEND` (see subroutine PARACO). Only lists of processors are necessary, regardless of any order in the communications, the rest is handled by MPI. To achieve this, a number of new data have been added to the `BIEF_MESH` structure. They are listed below. Moreover in version 5.9 parallel communication data linked to segments have been added, which doubles the necessary data.

NB_NEIGHB number of neighbouring processors (seen by points).

NB_NEIGHB_SEG number of neighbouring processors (seen by segments).

NB_NEIGHB_PT number of points shared with processors (array of size NB_NEIGHB).

NB_NEIGHB_PT_SEG number of segments shared with processor I (array of size NB_NEIGHB_SEG).

LIST_SEND list of neighbouring processors to which data must be sent (seen by points).

LIST_SEND_SEG list of neighbouring processors to which data must be sent (seen by segments).

There should be also accordingly a LIST_RECEIVE, but it is actually exactly like LIST_SEND, so it has not been created.

NH_COM array of size (DIM1_NHCOM,NB_NEIGHB). DIM1_NHCOM is at least the maximum number of points that can be shared with a single processor. It can be slightly more for optimisation (see subroutine PARINI). NH_COM(I,J) is the global number in the subdomain of the I^{th} point shared with the J^{th} neighbouring processor.

NH_COM_SEG like NH_COM but for segments.

BUF_SEND buffer of memory that will be used by MPI subroutines.

BUF_RECV buffer of memory that will be used by MPI subroutines.

Specific cases

It is worth noting that just a few alterations of the scalar and matrix-vector products are sufficient to solve a linear equation with partial derivative in shared memory. Furthermore, the contributions of the interfacial terms can be postponed until the final solving. They would be necessary before only if real nodal values, dot product, matrix-vector product or final results are needed. For a linear equation, these operations can be confined in the resolution of the linear system. Once the tools have been set up to communicate between processors, parallelization of fluid mechanics software is quite easy. However, specific cases, arising mainly from nonlinearity have to be considered. The basic idea is to get identical results on vector or parallel computers, except for truncation errors. Some examples follow:

- Diagonal preconditioning: the diagonal used for preconditioning has to be completed at the interfaces.

- Computation of nodal values after projection onto a basis: let us consider the gradient of a function f. A mean nodal value of $\overrightarrow{grad}(f)$ is given by:

$$\overrightarrow{grad}(f)_i = \frac{\int_\Omega \overrightarrow{grad}(f)\Psi_i d\Omega}{\int_\Omega \Psi_i d\Omega}$$

  issued from the mean-value theorem. In this case the computation of the general term $\int_\Omega \Psi_i d\Omega$ has to be completed at the interfaces. The vector including: $\int_\Omega \overrightarrow{grad}(f)\Psi_i d\Omega$ is unchanged when added to the right-hand side of a linear system (the solver itself will complete this term). However it must be completed when used to compute another term such as a turbulent production.

- any global concept: maximum Courant number, maximum Froude number, etc., have to be transmitted between processors.

- the method of characteristics: for high values of the Courant number, a characteristic curve may leave a sub-domain and enter others. Programming this situation within the parallel architecture requires a huge number of random transmissions, depending on the flow. The implementation of this technique in parallel has been achieved by Jacek Jankowski from BundesAnstalt für Wasserbau in Germany.

4.7 Utilities

A number of tools are offered in BIEF, in the form of functions and subroutines.

4.7.1 Functions

All the functions described below facilitate programming and avoid transmission of arguments.
syntax:

```
INTEGER FUNCTION DIMENS(IELM)
```

IELM is a type of element. DIMENS returns the dimension corresponding to the element given. For example, DIMENS(11) = 2.
syntax:

```
DOUBLE PRECISION FUNCTION DOTS(T1,T2)
```

T1 and T2 may be two vectors, or two blocks.
For vectors, returns their scalar product. For blocks, returns the sum of the scalar products of the vectors they contain.

> **Warning:**
> Only the first dimension of the vectors is taken into account for the time being.

See also `P_DOTS`
syntax:

```
LOGICAL FUNCTION EOF(LUNIT)
```

LUNIT is the logical function of a file. EOF says if we are at the end of this file or not.
syntax:

```
INTEGER FUNCTION IELBOR(IELM,I)
```

Returns the type of boundary element associated with a given element. For example, IELBOR(11,1) = 1. I is used when there are several types of boundary elements. For a prism, for example, IELBOR(41,1)=11 and IELBOR(41,2)=21.
syntax:

```
INTEGER FUNCTION BIEF_NBFEL(IELM,MESH)
```

Returns the number of faces for the element type IELM (value initialised in `BIEF_ININDS`)
syntax:

```
INTEGER FUNCTION BIEF_NBPEL(IELM,MESH)
```

Returns the number of points per element for the element type IELM. (value initialised in `BIEF_ININDS`). Though MESH is an argument, it is not function of the mesh.
syntax:

```
INTEGER FUNCTION BIEF\_NBMPTS(IELM,MESH)
```

Returns the maximum number of points in the domain for a given discretisation, in the case of an adaptive mesh. For the time being, this function is equal to BIEF_NBPTS.
syntax:

```
INTEGER FUNCTION BIEF_NBPTS(IELM,MESH)
```

Returns the number of points in the domain for a given discretisation (value initialised in `BIEF_ININDS`) and a given mesh.
syntax:

```
INTEGER FUNCTION BIEF_NBSEG(IELM,MESH)
```

Returns the number of segments in the domain for a given discretisation (value initialised in `BIEF_ININDS`) and a given mesh.
syntax:

```
INTEGER FUNCTION BIEF_NBSEGEL(IELM,MESH)
```

Returns the number of segments of an element for a given discretisation (value initialised in `BIEF_ININDS`). Actually does not depend on the mesh.
syntax:

```
DOUBLE PRECISION FUNCTION P_DOTS(T1,T2,MESH)
```

As DOTS but takes into account domain decomposition. `P_DOTS` will thus communicate with other processors to get their contribution.
MESH is the mesh structure.

Warning:
Only the first dimension of the vectors is taken into account for the time being.

syntax:

```
DOUBLE PRECISION FUNCTION BIEF_SUM(T1)
```

T1 may be a vector, or a block.
For a vector, returns the sum of the vector components. For a block, returns the sum of all the components of the vectors it contains.

Warning:
Only the first dimension of the vectors is taken into account for the time being.

syntax:

```
INTEGER FUNCTION TIME_IN_SECONDS()
```

Returns the time in seconds given by the computer clock. For computing the elapse time of a job. Beware, this value is sometimes reset to zero by the computer, generally every 24 hours.

4.7.2 Basic subroutines

syntax:

```
SUBROUTINE BIEF\_CLOSE\_FILES(CODE,FILES,NFILES,PEXIT
```

Replaces the old `CLOSE_FILES` or `CLOSE_FILES2`
arguments:

CODE is a 20 characters string saying which programme calls the subroutine, for example 'ARTEMIS'.

FILES is an array of `BIEF_FILE` structures containing a description of all files used by the program.

NFILES is the number of files (and dimension of FILES)

PEXIT is a logical value. If yes, the call to the subroutine will also trigger an exit from MPI.

All the relevant files, whose names are known through the DECLARATIONS_TELEMAC module, are closed by this subroutine.
syntax:

```
SUBROUTINE CLIP(VEC,XMIN,CLPMIN,XMAX,CLPMAX,NPOIN)
```

arguments:

CLIP clips an array of real values:

- Lower values limited by XMIN if the logic CLPMIN is true.
- Upper values limited by XMAX if the logic CLPMAX is true.

CLIP can handle vector structures as well as conventional FORTRAN arrays.

NPOIN For a conventional array, NPOIN is taken as a dimension of the array.

VEC must be a BIEF_OBJ structure of vector type:

- If NPOIN = 0, the dimension given by the structure is taken.
- If NPOIN<0, the dimension -NPOIN is imposed. This must then be less than or equal to the real dimension.

syntax:

```
SUBROUTINE FILTER( VEC,BLDMAT,T1,T2,A,FORMUL,XMUL,F,G,H,U,V,W,MESH,MSK,MASKEL,N)
```

Filtering operation of the vector VEC. T1 and T2 are working BIEF_OBJ structures. From XMUL, the arguments are the same as those of MATRIX. A is a matrix which is either given (if the logical value BLDMAT is false), or constructed according to the formula FORMUL (if BLDMAT is true). In the latter case, the arguments F, G, H, U, V, W, may be used if they appear in the formula FORMUL.
VEC is modified **N times** by FILTER according to the following formula: $newVEC = XMUL * \frac{A*VEC}{A^L}$ where A^L is the diagonal matrix obtained by mass-lumping A, that is by totalling the terms in each row.

If A is a mass matrix (FORMUL = 'MATMAS '), a smoothed vector VEC is obtained, with its integral in the domain (the 'mass') preserved.
If FORMUL = 'FMATMA ', a smoothed vector VEC is obtained, with preservation of the integral of the function F VEC.
syntax:

```
SUBROUTINE BIEF_OPEN_FILES(CODE,FILES,NFILES,PATH,FLOT,IFLOT,ICODE)
```

Replaces the old `OPEN_FILES`, to enable coupled programs to run concurrently even if they use the same logical units.
The first three arguments are like `BIEF_CLOSE_FILES`.
PATH is the full name of the path leading to the directory containing the files (or at least the parameter file).
FLOT is a logical value stating if there is code coupling. In this case the logical units of every file are dynamically computed and will start at IFLOT+1, IFLOT being the argument after FLOT.
IFLOT: see explanations on FLOT above.
ICODE is the code number in case of coupling (the calling program will be code 1, the called program will be code 2).
The basic data for opening the files is stored in the dictionary of each program, namely in the key-word called SUBMIT. Here is the example for the geometry file in TELEMAC-2D:
SUBMIT : 'NGEO-READ;T2DGEO;OBLIG;BIN;LIT;SELAFIN-GEOM'
NGEO is no longer used.
READ means that this file will be opened in only read mode.
T2DGEO will be the name of the file in the temporary directory where the case will be run. T2DGEO is also declared in TELEMAC-2D as an integer which is the file number. It will be 1 and will not float in case of code coupling.
OBLIG means that the file is mandatory
BIN means that it is a binary file
LIT is a message for parallelism that the file will be read by every processor and must thus be copied for every of them. ECR would mean that it is a result that must be given back with an extension indicating the processor number.
SELAFIN-GEOM indicates that the file is at the SELAFIN format and GEOM says that it must be taken as the geometry file for domain decomposition. Other possibilities are : CAS (steering file), DICO (dictionary), CONLIM (boundary conditions to be taken into account in domain decomposition).
All the possibilities are documented in the dictionaries of parallelised programs.
The last argument ICODE is the program number in case of coupling. So far some data in BIEF library are concurrently used by coupled programs, hence BIEF must now which program is running, this is done by using: `CALL CONFIG_CODE(ICODE)` when shifting to another program in code coupling, `CONFIG_CODE` will thus avoid conflicts between files.
Note : the parameter file and the dictionary have prescribed names and are not opened by `BIEF_OPEN_FILES`. For example, in TELEMAC-2D they are opened and closed in subroutine LECDON_TELEMAC2D.
syntax:

```
SUBROUTINE PARCOM(X,ICOM,MESH)
```

PARCOM completes the matrix-vector product in parallelism, by adding to a vector X contributions from elements that are in other sub-domains.
Arguments:

X is a BIEF_OBJ structure of a vector or a block of vectors.

ICOM is an option.

- ICOM = 1: the contribution with maximum absolute value is taken.
- ICOM = 2: the sum of contributions is taken (the most widely used option).
- ICOM = 3: the maximum value is taken.
- ICOM = 4: the minimum value is taken.

MESH is the BIEF_MESH structure of the mesh.

This subroutine is able to work in 2D and 3D as well. Blocks of vectors are also treated. In 2D it will also cope with quadratic discretisation, which implies not only a communication of points, but also of segments. PARCOM calls a subroutine `PARCOM2` and a subroutine `PARCOM2_SEG` which act directly on real vectors. The call to PARCOM may be bypassed in specific cases, e.g. when a parallel communication of segments is required.
syntax:

```
SUBROUTINE PARMOY(X,MESH)
```

`PARMOY` is used in parallelism to give the mean value of a vector X at the interface between 2 sub-domains. MESH is the `BIEF_MESH` structure of the mesh.

4.7.3 Subroutines dealing with the selafin format file

T his section is obsolete since v7p1 due to the introduction of hermes See Chapter 9 for information on Hermes.

The SELAFIN format is used in 2D and 3D for the results files and for the geometry files. It is given in appendix 3. Several routines are offered for writing or reading such files. Others remain internal routines in BIEF and will be called directly either by ALMESH or INBIEF.
syntax:

```
SUBROUTINE ECRGEO(X,Y,NPOIN,NBOR,NFIC,NVAR,TEXTE,VARCLA,
                  NVARCL,TITRE,SORLEO,NSOR,IKLE,NELEM,
                  NPTFR,NDP,DATE,TIME,NCSIZE,NPTIR,KNOLG)
```

arguments:

X,Y are the coordinates of the mesh (equivalent to MESH%X%R and MESH%Y%R)

NPOIN is the number of nodes in the mesh

NBOR is the array MESH%NBOR%I giving the global numbers of boundary points.

NFIC is the logical unit of the file

NVAR is the number of variables to write in the file (at every time-step)

TEXTE is the 32 characters strings given the names and units of variables (SORLEO, see below, will say if they must be put in the file).

VARCLA is another array of 32 characters strings used for the so-called clandestine variables in TELEMAC-2D, i.e. variables which are in the geometry file and are merely transmitted to the results file.

NVARCL is the number of clandestine variables.

TITRE is the title of the file or the study (80 characters).

SORLEO is an array of logical values saying which variables in the list TEXTE will be put in the file.

NSOR is the size of SORLEO

IKLE , NELEM, NPTFR, NDP are the classical components of BIEF_MESH structures : connectivity table, number of elements, number of boundary points and number of points per element.

DATE and TIME are two arrays of 3 integers giving the year, month, day and hour, minute, second

NCSIZE is the number of processors.

NPTIR is the number of interface points with other sub-domains (if NCSIZE greater than 1).

KNOLG is the global number of points in the original mesh (if NCSIZE greater than 1).

syntax:

```
SUBROUTINE FILPOL(F,C,XSOM,YSOM,NSOM,MESH)
```

arguments:

FILPOL fills a vector F with a constant C, but only for points of F which are in a given polynomial in the computational domain.

F is a BIEF_OBJ structure of a vector.

C is the constant.

XSOM and YSOM are arrays of double precision numbers giving the coordinates of the apices of the polynomial.

NSOM is the number of apices (e.g. 3 for a triangle).

MESH is the BIEF_MESH structure of the mesh.

syntax:

```
SUBROUTINE FIND\_IN\_SEL(RES,NAME,NFIC,W,OK)
```

FIND_IN_SEL will find in a SELAFIN format file a variable with a given name.
arguments:

RES is a BIEF_OBJ structure to put the result in.

NAME is the name of the variable (16 characters).

NFIC is the logical unit of the file

W is a working real (real, not double precision) array of size the number of points in the mesh.

OK is a logical value saying if the variable has been found.

syntax:

```
SUBROUTINE FONSTR( H,ZF,Z,CHESTR,NGEO,NFON,NOMFON,MESH,FFON,LISTIN)
```

FONSTR can find the bottom topography and the bottom friction in a geometry file in the SELAFIN format. In this file the bottom topography must be called FOND or BOTTOM, the friction must be called FROTTEMENT or BOTTOM FRICTION. If the bottom is not in the file, another possibility is that the bottom is computed as a function of the free surface and the depth. In this case they must be called respectively SURFACE LIBRE or FREE SURFACE and HAUTEUR D'EAU or WATER DEPTH. The bottom can also be given as a cluster of bathymetry points in a specific file. These data will then be interpolated to give nodal values. The format of bathymetry points is the following: every line is dedicated to 1 point with X Y Z in free format. Xand Y are the coordinates and Z is the bottom elevation.
Lines beginning with C or B are ignored. With such a standard, SINUSX files can be read.
If the bottom friction is not in the geometry file, CHESTR is set to the value FFON.
The arguments of FONSTR are:

H,ZF,Z are BIEF_OBJ structures where the depth (if any), the bottom, and the free surface (if present) will be stored.

CHESTR is the BIEF_OBJ structure for the friction coefficient.

NGEO is the logical unit of the geometry file.

NFON is the logical unit of the bottom file.

NOMFON is the name of the bottom file.

MESH is the BIEF_MESH structure of the mesh.

FFON is the friction coefficient if it is constant.

LISTIN is a logical value. If yes, information will be printed.

The bottom friction can then be changed with the user subroutine STRCHE.
syntax:

```
SUBROUTINE LITENR(VARSOR,CLAND,NPRE,STD,HIST,NHIST,NPOIN,
                  AT, TEXTPR, TEXTLU, NVAR, VARCLA, NVARCL,
                  TROUVE, ALIRE, W, LISTIN, MAXVAR)
```

LITENR will read a time record in a selafin file. It assumes that the heading with geometry data has been read, and that a number of time records may also have been read. Some variables of the next time record are read by LITENR. As in ECRGEO, the name of variables is in TEXTPR, but in this list, only the variables given by the logical array ALIRE will be read. The result will be put in a block called VARSOR. If there are clandestine variables (their number is NVARCL), their name is given in VARCL and they will be put into the block CLAND. Other arguments are:

NPRE logical unit of the file.

STD binary standard of the file (3 characters STD, IBM or I3E). Obsolescent, use 'STD'.

HIST sometimes an array of real values may be put after the time in the same record.

NHIST size of NHIST. So far 0 because it is not implemented in RUBENS.

NPOIN number of points in the mesh.

AT time of the record read by LITENR.

TEXTLU is a working array of character*32 strings to store the names of variables in the file.

NVAR is the number of normal variables

TROUVE is an integer array saying if the variables asked have been found.

W : s a working real (real, not double precision) array of size the number of points in the mesh.

LISTIN is a logical saying if information on what is read must be printed.

syntax:

```
SUBROUTINE SKIPGEO(NFIC,TITFIC,NPOIN,NVAR,TEXTLU
```

SKIPGEO reads a SELAFIN file with logical unit NFIC up the time records. It returns the title of the file: TITFIC, the number of points in the mesh: NPOIN, the number of variables stored: NVAR, and their names and units: TEXTLU (an array of CHARACTER*32 strings).

4.7.4 Subroutines dealing with all formats

From version 6.2 on several formats are accepted for inputs and outputs and new subroutines have been created to deal with this new feature. For example the equivalent of the former `ECRGEO` with be a sequence of a call to `CREATE_DATASET` and a call to `WRITE_MESH`. Writing a record of results will be done with `BIEF_DESIMP` (which also prints on the listing) or `WRITE_DATA`.
syntax:

```
SUBROUTINE BIEF_DESIMP( FORMAT_RES, VARSOR, HIST, NHIST,
                        N, NRES, STD, AT, LT, LISPRD, LEOPRD,
                        SORLEO, SORIMP, MAXVAR, NOMVAR, PTINIG, PTINIL )
```

arguments:

FORMAT_RES is the file format ('SELAFIN ', 'SELAFIND' or 'MED ')

VARSOR is a block containing BIEF_OBJ structures with the variables to be printed in the file.

HIST and NHIST are used to add data in the time record of the Selafin format (HIST will be the array of the values and NHIST their number)

N is the number of points to be printed (it may be different from the number of degrees of freedom, as some values are dropped when quasi-bubble or quadratic elements are used).

NRES is the logical unit of the file.

STD is a 3-character string (meant for binary variants, currently not used)

AT is the current time.

LT is the iteration number.

LISPRD and LEOPRD are the printing periods on listing and file.

SORLEO and SORIMP are logical arrays stating if a variable must be exited or not (same order as in the block VARSOR).

MAXVAR is the number of variables in the block VARSOR, and the dimension of SORLEO and SORIMP.

NOMVAR is an array of 32-character strings containing the names (16 characters) and units (16 characters) of variables.

PTINIG and PTINIL are the time steps (respectively for file and listing) at which will start the prints. These integers stem from key-words such as `NUMBER OF FIRST TIME-STEP FOR GRAPHIC PRINTOUTS` in TELEMAC-2D and TELEMAC-3D.

syntax:

```
SUBROUTINE BIEF_SUITE(VARSOR, CLAND, NUMDE, NPRE, STD,
                      HIST, NHIST, NPOIN, AT, TEXTPR,
                      VARCLA, NVARCL, TROUVE, ALIRE,
                      LISTIN, FIN, MAXVAR, NPLAN, DT)
```

`BIEF_SUITE` is used to start a new computation from previous results. The time record to start with is the last one if FIN=.TRUE., and is NUMDEB if FIN=.FALSE. Otherwise the principle and arguments are the same as LITENR, see above. For Selafin format `BIEF_SUITE` is a combination of SKIPGEO and LITENR.
NPLAN and DT are optional parameters.
If NPLAN is present (case of TELEMAC-3D with prisms) and if the number of planes is different, the data will be interpolated to cope with the number of planes asked, i.e. NPLAN.
If DT is present, the time step of records in the file will be returned. This assumes that there are at least 2 records in the file, otherwise an error message will be issued.
syntax:

```
SUBROUTINE BIEF_VALIDA(VARREF, TEXTREF, UREF, REFFORMAT, VARRES,
                       TEXTRES, URES, RESFORMAT, MAXTAB, NP, IT,
                       MAXIT, ACOMPARER)
```

BIEF_VALIDA offers an automatic way to compare two SELAFIN files to perform validations of modifications in a program. A reference file (logical unit UREF) is compared to a result file (logical unit URES).
VARREF and VARRES are blocks where the variables to read will be put.
TEXTREF and TEXTRES are the names of the variables and give their implicit numbering.
UREF and URES are the logical units of reference file and result file.
REFFORMAT and RESFORMAT are the formats of reference file and result file (i.e. 'SELAFIN ','SELAFIND' or 'MED '.
MAXTAB is the maximum number of variables.
NP the number of points in the mesh.
IT and MAXIT are respectively the current and the maximum iteration. A comparison is done only when the last iteration MAXIT is reached and only the last time-step is checked.
ACOMPARER is an integer array saying if a variable must be checked (1) or not (0).
syntax:

```
SUBROUTINE CREATE_DATASET(FORMAT,NRES,TITLE,MAXVAR,NOMVAR,OUTVAR)
```

FORMAT: a 8-character string. Possible values are 'SELAFIN ', 'SELAFIND' and 'MED '. SELAFIN is the classical format in the Telemac system. SELAFIND is the same but with real numbers saved in double precision (so far not supported by post processors). MED is an EDF format that is recognised by all tools of the Salome platform.
NRES: the logical unit
In TELEMAC-2D for example and for the results file, these first two arguments will be:
T2D_FILES(T2DRES)%FMT and T2D_FILES(T2DRES)%LU.
TITLE is the title of the case, in 80 characters.
MAXVAR is the maximum number

This subroutine will only store in the file the information of the title and the names and units of variables.
syntax:

```
SUBROUTINE WRITE\_DATA(FORMAT_RES, NRES, MAXVAR, AT,
                       LT, SORLEO, NOMVAR, VARSOR, N)
```

Mostly as BIEF_DESIMP, but a lower level. It will not deal with periods and printing on listing.
arguments:

FORMAT_RES is the file format ('SELAFIN ', 'SELAFIND' or 'MED ')

NRES is the logical unit of the file.

MAXVAR is the number of variables in the block VARSOR and NOMVAR.

AT is the current time, LT is the iteration number.

SORLEO is a logical array stating if a variable must be exited or not.

NOMVAR is an array of 32-character strings containing the names (16 characters) and units (16 characters) of variables.

VARSOR is a block containing BIEF_OBJ structures with the variables to be printed in the file.

N is the number of points to be printed.

syntax:

```
SUBROUTINE WRITE_MESH(FORMAT, NRES, MESH, NPLAN, MARDAT,
                      MARTIM, I_ORIG, J_ORIG)
```

arguments:

FORMAT and NRES are like in subroutine `CREATE_DATASET` above.

MESH is the BIEF_MESH structure of the mesh.

NPLAN is the number of planes in the mesh (1 in 2D).

MARDAT and MARTIM are two arrays of 3 integers containing the date : year, month, day, and hours, minutes, seconds.

I_ORIG and J_ORIG are the numbers of metres to add to coordinates to get georeferenced data.

4.7.5 Scientific library

Some scientific functions have been included in BIEF for convenience:
syntax:

```
DOUBLE PRECISION FUNCTION ATANC(A,B)
```

ATANC returns the Arc tangent of A.
syntax:

```
DOUBLE PRECISION FUNCTION JULTIM(YEAR,MONTH,DAY,HOUR,MIN,SEC,AT)
```

JULTIM returns the time in Julian centuries since the 31 December 1899. The starting time of a computation is given by YEAR,MONTH,DAY,HOUR,MIN,SEC, and AT (current time in the computation is added).
syntax:

```
DOUBLE PRECISION FUNCTION TSLOC(YEAR,MONTH,DAY,HOUR,MIN,SEC,AT)
```

TSLOC returns the local sidereal time.

4.7.6 Higher order subroutines in BIEF

A number of subroutines in BIEF are more dedicated to physics and can be directly called by programmes to solve e.g. diffusion or advection equations:
syntax:

```
SUBROUTINE CVDFTR
```

In 2 dimensions, solves the advection-diffusion of a tracer, including source terms. Starting from a tracer FN at time step n, it gives back the tracer F at time step n+1. Refer to source code for a full list of arguments. The advection may have been done previously by the method of characteristics, in which case the result is in `FTILD`, or is done by `CVDFTR` itself, which may call other subroutines such as `CVTRVF` and `CVTRVF_POS`. Explicit and implicit source terms may be treated, as well as punctual sources. An argument `ICONVF` monitors the choice of the advection scheme.
syntax:

```
SUBROUTINE CHARAC
```

This is the header subroutine for advection with the method of characteristics. It calls scalar or parallel variants of this method. The parallel version of the method of characteristics is included in module `STREAMLINE`. `CHARAC` may deal with a single.
Refer to source code for a full list of arguments. FN is the variable to be advected and FTILD the result. They may be blocks of variables and in this case the argument NOMB is the number of variables that will be treated.

4.7.7 User subroutines in BIEF

A number of subroutines are called by BIEF and may be changed by the user to implement specific cases. These subroutines have generally no arguments and only global data defined in a module may thus be changed. Subroutines are provided with examples.
syntax:

```
SUBROUTINE CORLAT
```

CORLAT is called by INBIEF when the coordinates are spherical. It allows changing of latitude and longitude of points.
syntax:

```
SUBROUTINE CORRXY
```

CORRXY is called once at the beginning of INBIEF (and before CORLAT). It allows to change the coordinates of points. Users are free to do any change (for example translations or rotations) provided that it keeps the topology of the mesh.
A translation in TELEMAC-2D would be done by adding `USE DECLARATIONS_TELEMAC2D` in `CORRXY`, declaring integer I, and then:

```
DO I=1,NPOIN
  X(I) = X(I) + 100.D0
```

```
  Y(I) = Y(I) + 200.D0
ENDDO
```

As a matter of fact, NPOIN, X and Y are pointers defined in `DECLARATIONS_TELEMAC2D`, to `MESH%NPOIN`, `MESH%X%R` and `MESH%Y%R`
syntax:

```
SUBROUTINE STRCHE
```

`STRCHE` is called once after reading the bottom friction in the geometry file, or after setting it to a constant value. This subroutine is empty and can be used only with modules containing global declarations. We give hereafter an example that would work with TELEMAC-2D:

```
SUBROUTINE STRCHE
  USE BIEF
  USE DECLARATIONS_TELEMAC2D
  INTEGER I
  DO I=1,NPOIN
    IF(X(I).GT.5.D0) THEN
      CHESTR%R(I) = 35.D0
    ELSE
      CHESTR%R(I) = 30.D0
    ENDIF
  ENDDO
  RETURN
END
```

4.8 Designing a new programme

4.8.1 Global data

Global data are defined by Fortran 90 modules. A number of other data are gathered in a BIEF module called `DECLARATIONS_TELEMAC`. It is given below:

```
!
!  DECLARATIONS COMMON TO ALL PROGRAMMES      VERSION 6.1
!
      MODULE DECLARATIONS_TELEMAC
!
!----------------------------------------------------------------------
!
! 1./ INTEGER VALUES FOR DESCRIBING BOUNDARY CONDITIONS:
!
!     FOR THE BOUNDARY CONDITIONS FILE:
!
!     ENTRANCE: PRESCRIBED VALUES (SAVE VELOCITIES)
      INTEGER, PARAMETER :: KENT  =  5
!
!     VELOCITY IMPOSED (INSTEAD OF DISCHARGE)
      INTEGER, PARAMETER :: KENTU =  6
!
!     FREE OUTPUT
      INTEGER, PARAMETER :: KSORT =  4
!
!     NO-SLIP CONDITION
      INTEGER, PARAMETER :: KADH  =  0
!
!     WALL WITH OR WITHOUT FRICTION
```

```
      INTEGER, PARAMETER :: KLOG  =  2
!
!     OPEN BOUNDARY WITH INCIDENT WAVE
      INTEGER, PARAMETER :: KINC  =  1
!
!     ESTEL-2D : DRAINAGE LIBRE
      INTEGER, PARAMETER :: KDRAIN  =  3
!
!     ESTEL-2D : CONDITION MIXTE
      INTEGER, PARAMETER :: KMIX  =  4
!
!     DEPENDING ON ALGORITHMS AND CASES, THESE VALUES WILL BE TRANSFORMED
!     INTO:
!
!     TECHNICAL BOUNDARY CONDITIONS
!
!     NEUMANN
      INTEGER, PARAMETER :: KNEU  =  1
!
!     DIRICHLET
      INTEGER, PARAMETER :: KDIR  =  2
!
!     DEGREE OF FREEDOM
      INTEGER, PARAMETER :: KDDL  =  3
!
!     INCIDENT WAVE
      INTEGER, PARAMETER :: KOND  =  4
!
!-----------------------------------------------------------------------
!
! 2./ CODE COUPLING
!
      CHARACTER*144 COUPLING
!
! 3./ NAME OF CURRENT CODE (SEE BIEF_OPEN_FILES AND CONFIG_CODE)
!
      CHARACTER(LEN=24) :: NNAMECODE(3)
!
!-----------------------------------------------------------------------
!
      END MODULE DECLARATIONS\_TELEMAC
```

To use these values, it is only necessary to write:

```
USE DECLARATIONS\_TELEMAC
```

as the first statement of every program or subroutine using them.
It is recommended to do a module of global declarations of your programme, containing the data read in the parameter file, the BIEF_OBJ structures, etc. However this module must not be used in subroutines that would be called by another programme in the Telemac system, which has no such declarations.

4.8.2 General structure of a programme based on BIEF 6.1

Main program

We give hereafter *in extenso* the example of the main program of TELEMAC-2D, which exemplifies all complex cases: parameter estimation and code coupling.

```
!                        ***********************
                         PROGRAM HOMERE_TELEMAC2D
!                        ***********************
!
!***********************************************************************
!  TELEMAC 2D VERSION 6.2   27/03/09  J-M HERVOUET (LNHE) 01 30 87 80 18
!
!***********************************************************************
!
!     FONCTIONS:
!     ==========
!
! 1)   READING ALL NECESSARY DATA
!
! 2)   CALLING TELEMAC2D AND IN CASE OF COUPLING SISYPHE
!
!     IN CASE OF PARAMETER ESTIMATION, HOMERE_ADJ_T2D IS CALLED INSTEAD
!     TELEMAC2D
!
!-----------------------------------------------------------------------
!
! APPELE PAR : PRINCI
!
! SOUS-PROGRAMMES APPELES : LECDON , POINT , TELEMAC2D
!
!**********************************************************************
!
      USE BIEF
      USE DECLARATIONS_TELEMAC
      USE DECLARATIONS_TELEMAC2D
      USE DECLARATIONS_SISYPHE, ONLY : SIS_FILES
      USE INTERFACE_TELEMAC2D
!
      IMPLICIT NONE
      INTEGER     LNG,LU
      COMMON/INFO/LNG,LU
!
      INTEGER TDEB(8),TFIN(8),NCAR,IFLOT
!
      CHARACTER(LEN=24), PARAMETER :: CODE1='TELEMAC2D               '
      CHARACTER(LEN=24), PARAMETER :: CODE2='SISYPHE                 '
!
      CHARACTER(LEN=250) PATH
      CHARACTER(LEN=144) MOTCAR(300),FILE_DESC(4,300)
!
!======================================================================
!
!     INITIALISING FILES (NAMES OF FILES=' ' AND LOGICAL UNITS =0)
!     GETTING NCSIZE BY CALLING P_INIT
!
      CALL BIEF_INIT(CODE1,PATH,NCAR,.TRUE.)
!
!     INITIAL TIME FOR COMPUTATION DURATION
!
      CALL DATE_AND_TIME(VALUES=TDEB)
!
```

```
!     PRINTING BANNER ON LISTING
!
      IF(LNG.EQ.1) WRITE (LU,100)
      IF(LNG.EQ.2) WRITE (LU,101)
      WRITE (LU,102)
100   FORMAT(/////,1X,'LISTING DE TELEMAC-2D ',78('-'))
101   FORMAT(/////,1X,'LISTING OF TELEMAC-2D ',78('-'))
102   FORMAT(/////,
     &14X,'    TTTTT  EEEEE  L      EEEEE  M   M  AAAAA  CCCCC',/,
     &14X,'      T    E      L      E      MM MM  A   A  C    ',/,
     &14X,'      T    EEE    L      EEE    M M M  AAAAA  C    ',/,
     &14X,'      T    E      L      E      M   M  A   A  C    ',/,
     &14X,'      T    EEEEE  LLLLL  EEEEE  M   M  A   A  CCCCC',/,
     &14X,'                                                   ',/,
     &14X,'           2D     VERSION 6.0     FORTRAN 90       ',/,
     &14X,'                  WITH SEVERAL TRACERS             ',/,
     &14X,'           COUPLED WITH SISYPHE INTERNALLY         ',/,
     &14X,/////)
!
!-----------------------------------------------------------------------
!
!     READING THE STEERING FILE
!
      CALL LECDON_TELEMAC2DLECDON_TELEMAC2D(MOTCAR,FILE_DESC,PATH,NCAR)
!
!-----------------------------------------------------------------------
!
!     OPENING FILES FOR TELEMAC2D
!
      IFLOT = 0
      CALL BIEF_OPEN_FILESBIEF_OPEN_FILES(CODE1,T2D_FILES,44,PATH,NCAR,
     &                          INCLUS(COUPLING,'INTER'),IFLOT,1)
!
!-----------------------------------------------------------------------
!
!     MEMORY ALLOCATION
!
      CALL POINT_TELEMAC2DPOINT_TELEMAC2D
!
!     SAVING COMMON NDS CORRESPONDING TO TELEMAC-2D MESH
!
      CALL SAVE_NDS(1)
!
!-----------------------------------------------------------------------
!
!     INITIALISING SISYPHE
!
      IF(INCLUS(COUPLING,'SISYPHE')) THEN
!
!                                               FALSE= P_INIT NOT CALLED
        CALL BIEF_INIT(CODE2,PATH,NCAR,.FALSE.)
!
        IF(LNG.EQ.1) WRITE (LU,103)
        IF(LNG.EQ.2) WRITE (LU,104)
        WRITE (LU,105)
103     FORMAT(/////,1X,'LISTING DE SISYPHE AVEC COUPLAGE',78('-'))
```

```
104     FORMAT(/////,1X,'LISTING OF SISYPHE WITH COUPLING',78('-'))
105     FORMAT(/////,
     &  14X,'    SSSS I   SSSS Y   Y PPPP  H   H EEEEE' ,/,
     &  14X,'   S     I  S      Y Y  P   P H   H E    ' ,/,
     &  14X,'    SSS  I   SSS    Y   PPPP  HHHHH EEEE  ',/,
     &  14X,'       S I     S   Y   P     H   H E     ',/,
     &  14X,'   SSSS  I  SSSS    Y   P     H   H EEEEE' ,/,
     &  14X,'                                          ',/,
     &  14X,'                VERSION 6.0               ',/,
     &  14X,'      COUPLED WITH TELEMAC-2D INTERNALLY  ',/,
     &  14X,/////)
!
      CALL LECDON_SISYPHE(MOTCAR,FILE_DESC,PATH,NCAR,CODE1)
!
      CALL BIEF_OPEN_FILESBIEF_OPEN_FILES(CODE2,SIS_FILES,44,PATH,NCAR,
     &                    INCLUS(COUPLING,'SISYPHE'),IFLOT,2)
      CALL POINT_SISYPHE
!
!     SAVING COMMON NDS CORRESPONDING TO SISYPHE MESH (SO FAR THE SAME !)
!
      CALL SAVE_NDS(2)
!
      ELSEIF(COUPLING(1:1).EQ.' ') THEN
!
!       NOTHING TO DO
!
      ELSEIF(INCLUS(COUPLING,'DELWAQ')) THEN
!
!       NOTHING TO DO
!
      ELSE
!       ERREUR
        IF(LNG.EQ.1) WRITE (LU,*) 'CAS DE COUPLAGE INCONNU : ',COUPLING
        IF(LNG.EQ.2) WRITE (LU,*) 'UNEXPECTED COUPLING CASE: ',COUPLING
        CALL PLANTE(1)
        STOP
      ENDIF
!
!     RESETTING TELEMAC2D CONFIGURATION
!
      CALL CONFIG_CODE(1)
!
!=======================================================================
!
      IF(ESTIME.EQ.' ') THEN
!
!-----------------------------------------------------------------------
!
!     NORMAL MODE: ONE CALL OF TELEMAC2D
!
      CALL TELEMAC2D(PASS=-1,ATDEP=0.D0,NITER=0,CODE='       ')
!
!-----------------------------------------------------------------------
!
      ELSE
!
```

```
!-----------------------------------------------------------------------
!
!         PARAMETER ESTIMATION MODE : CALLING HOMERE_ADJ_T2D
!
          CALL HOMERE_ADJ_T2D
!
        ENDIF
!
!=======================================================================
!
!       CLOSING FILES
!
        CALL BIEF_CLOSE_FILES(CODE1,T2D_FILES,44,.TRUE.)
!
        IF(INCLUS(COUPLING,'SISYPHE')) THEN
          CALL CONFIG_CODE(2)
          CALL BIEF_CLOSE_FILES(CODE2,SIS_FILES,44,.FALSE.)
        ENDIF
!
!-----------------------------------------------------------------------
!
        IF(LNG.EQ.1) WRITE (LU,10)
        IF(LNG.EQ.2) WRITE (LU,11)
10      FORMAT(1X,///,1X,'FIN NORMALE DU PROGRAMME',///)
11      FORMAT(1X,///,1X,'CORRECT END OF RUN',///)
!
!-----------------------------------------------------------------------
!
!       TIME OF END OF COMPUTATION
!
        CALL DATE_AND_TIME(VALUES=TFIN)
        CALL ELAPSE(TDEB,TFIN)
!
!-----------------------------------------------------------------------
!
        STOP
        END
```

Some explanations:

- The statement `USE BIEF` is given first because the module `DECLARATIONS_TELEMAC2D` contains declarations of `BIEF_OBJ` structures, for example the depth H or the mesh called `MESH`.
- The string CODE contains the name of the programme and will be used by BIEF subroutines such as `BIEF_OPEN_FILES` to open the relevant files. It implies that the `LECDON_TELEMAC2D` subroutine uses also the module `DECLARATIONS_TELEMAC` and correctly fills the names of the files.

Other calls are explained in the following paragraphs.

Reading the parameter file

This is done by the call to `LECDON_TELEMAC2D`. Such a subroutine must be written for every program in the system. LECDON_TELEMAC2D calls the subroutine `DAMOCLES` which returns the parameters read in the dictionary file and in the user parameter file. We give hereafter parts of `LECDON_TELEMAC2D` as an example:

```
      USE DECLARATIONS_TELEMAC
      USE DECLARATIONS_TELEMAC2D
!
      IMPLICIT NONE
      INTEGER LNG,LU
      COMMON/INFO/LNG,LU
!
      INTEGER I,K,NCSIZE,ERR,NCAR
      INTEGER NREJEX,NREJEY,NCOSUP,NREJEV,NCRITE
!
      CHARACTER*8 MNEMO(MAXVAR)
      CHARACTER(LEN=250) PATH,NOM_CAS,NOM_DIC
      CHARACTER(LEN=144) FILE_DESC(4,300)
!
!-----------------------------------------------------------------------
!
!     DECLARATION OF ARRAYS FOR CALLING DAMOCLES
!
      INTEGER, PARAMETER :: NMAX = 300
!
      INTEGER                ADRESS(4,NMAX),DIMENS(4,NMAX)
      DOUBLE PRECISION       MOTREA(NMAX)
      INTEGER                MOTINT(NMAX)
      LOGICAL                MOTLOG(NMAX)
      CHARACTER(LEN=144)     MOTCAR(NMAX)
      CHARACTER*72           MOTCLE(4,NMAX,2)
      INTEGER                TROUVE(4,NMAX)
      LOGICAL DOC
!
!
.........
!
!     INITIALISATIONS FOR CALLING DAMOCLES :
!
      DO 10 K=1,NMAX
        MOTCAR(K)(1:1)=' '
        DIMENS(1,K)  = 0
        DIMENS(2,K)  = 0
        DIMENS(3,K)  = 0
        DIMENS(4,K)  = 0
10    CONTINUE
!     IF YES WILL PRINT ALL DOCUMENTATION IN DICTIONARY
      DOC = .FALSE.
!
!-----------------------------------------------------------------------
!     OPENING PARAMETER FILE AND DICTIONARY
!-----------------------------------------------------------------------
!
      IF(NCAR.GT.0) THEN
!
        NOM_DIC=PATH(1:NCAR)//'T2DDICO'
        NOM_CAS=PATH(1:NCAR)//'T2DCAS'
!
      ELSE
!
        NOM_DIC='T2DDICO'
```

```
          NOM_CAS='T2DCAS'
!
        ENDIF
!
        OPEN(2,FILE=NOM_DIC,FORM='FORMATTED',ACTION='READ')
        OPEN(3,FILE=NOM_CAS,FORM='FORMATTED',ACTION='READ')
!
!-----------------------------------------------------------------------
!
        CALL DAMOCLE( ADRESS , DIMENS , NMAX   , DOC     , LNG    , LU ,
     &                MOTINT , MOTREA , MOTLOG , MOTCAR  , MOTCLE ,
     &                TROUVE , 2      , 3      , .FALSE. , FILE_DESC )
!
!-----------------------------------------------------------------------
!     FERMETURE DES FICHIERS DICTIONNAIRE ET CAS
!-----------------------------------------------------------------------
!
        CLOSE(2)
        CLOSE(3)
```

Remark: the names of the steering file and the dictionary, their logical units are here hard-coded. As they are closed after, logical units 2 and 3 may be re-used.
After calling `DAMOCLES`, the parameters are in the arrays MOTINT, MOTREA, MOTLOG and MOTCAR if they are (respectively) integers, double precision numbers, logical values or character strings. Their rank in the arrays is given by their index in the dictionary.

- ADRESS(1,*) is the addresses of integers in array MOTINT.
- ADRESS(2,*) is the addresses of double precision numbers in array MOTREA.
- ADRESS(3,*) is the addresses of logical values in array MOTLOG.
- ADRESS(4,*) is the addresses of strings in array MOTCAR.

For example the turbulence model is in TELEMAC-2D an integer with rank 7 in the dictionary. It is initialised as follows:

```
ITURB              = MOTINT( ADRESS(1, 7) )
```

The size of arrays is given by `DIMENS`, for example the array of prescribed free surfaces (index 31 of double precision numbers in the dictionary) in TELEMAC-2D is initialised by:

```
NCOTE   = DIMENS(2,31)
IF(NCOTE.NE.0) THEN
  DO K=1,NCOTE
   COTE(K) = MOTREA( ADRESS(2,31) + K-1 )
  ENDDO
ENDIF
```

As MOTCAR is declared as an array of `CHARACTER(LEN=144)` strings, it may be necessary to take only a part of them, as below:

```
TITCAS     = MOTCAR( ADRESS(4, 1) )(1:72)
```

Where `TITCAS` is declared as a `CHARACTER(LEN=72)` string.
Checking and modifications of key-words should be done only in `LECDON`.

Allocating memory

This is done in the subroutine called POINT_NAMEOFPROGRAMME. We give and comment hereafter parts of POINT_TELEMAC2D:

```
      USE BIEF
      USE DECLARATIONS_TELEMAC
      USE DECLARATIONS_TELEMAC2D !where all BIEF_OBJ structures are declared
!
!+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+
!
.
.  (Declarations and printing skipped), then:
.
!
!     DISCRETISATIONS TYPES
!
!     P0 and P1 discretisation
!
      IELM0 = 10*(IELMH/10)
      IELM1 = IELM0 + 1
!
! P1 Discretisation of boundaries
!
      IELB1 = IELBOR(IELM1,1)
!     Element with the greatest number of degrees of freedom
      IELMX=MAX(IELMU,IELMH,IELMT,IELMK,IELME)
!
!     TYPE OF STORAGE AND MATRIX-VECTOR PRODUCT
!
      CFG(1)  = OPTASS
      CFG(2)  = PRODUC
!
!=======================================================================
!
!     ALLOCATING THE MESH
!
      CALL ALMESH(MESH,'MESH   ',IELMX,SPHERI,CFG,T2D_FILES(T2DGEO)%LU,
     &              EQUA,I3=I3,I4=I4)
!     IF ORIGIN COORDINATES IN GEOMETRY FILE AND NOT IN PARAMETER FILE,
!     VALUES OF GEOMETRY FILE ARE TAKEN
      IF(I3.NE.0.AND.I_ORIG.EQ.0)  I_ORIG=I3
      IF(I4.NE.0.AND.J_ORIG.EQ.0)  J_ORIG=I4
!
!     EXAMPLE OF CREATION OF ALIASES
!
      IKLE  => MESH%IKLE
      X     => MESH%X%R
      Y     => MESH%Y%R
      NELEM => MESH%NELEM
!
!=======================================================================
!
!     EXAMPLE OF ALLOCATION OF A REAL ARRAY
!
      CALL BIEF_ALLVEC(1,U,'U     ',IELMU,1,1,MESH)
!
```

```
!      EXAMPLE OF ALLOCATION OF A BLOCK
!
       CALL ALLBLO(UNK,'UNK    ')
!      ADDING BIEF_OBJ STRUCTURES IN THE BLOCK UNK
       CALL ADDBLO(UNK,DH)
       CALL ADDBLO(UNK, U)
       CALL ADDBLO(UNK, V)

!      EXAMPLE OF ALLOCATION OF A MATRIX
!
       CALL BIEF_ALLMAT(AM2,'AM2    ',IELM1,IELM1,CFG,'Q',TYP,MESH)
!
!      ALLOCATING A BLOCK TB WITH 3 VECTORS CALLED T1, T2 AND T3
!
       CALL ALLBLO(TB ,'TB     ')
       CALL BIEF_ALLVEC_IN_BLOCK(TB,42,1,'T      ',IELMX,1,2,MESH)
!
!      ALIASES FOR THESE ARRAYS
!      T1, T2 AND T3 ARE DECLARED IN DECLARATIONS_TELEMAC2D AS FOLLOWS
!      TYPE(BIEF_OBJ), POINTER :: T1,T2,T3
!      ALIASES FOR T1, T2 AND T3
       T1 =>TB%ADR(1)%P
       T2 =>TB%ADR(2)%P
       T3 =>TB%ADR(3)%P
```

The real main programme

The main program `HOMERE_...` given above calls `TELEMAC2D`. This is where the real specific job of your programme must be done. At the beginning of it, but after reading the boundary conditions file, the `BIEF_MESH` structure called MESH must be fully initialised, and this is done by a call to `INBIEF`:

```
       CALL INBIEF(LIHBOR%I,KLOG,IT1,IT2,IT3,LVMAC,IELMX,
      &             LAMBD0,SPHERI,MESH,T1,T2,OPTASS,PRODUC,EQUA)
```

Inputs and outputs: opening and closing files

The various data and results files of every Telemac programme are described in its dictionary. The information relevant to files will be read with the subroutine `READ_SUBMIT`, which is called in subroutine `LECDON_TELEMAC2D` (for example), and stored in an array of file structures (called, depending of the Telemac module: `T2D_FILES`, `T3D_FILES`, `SIS_FILES`, `WAC_FILES`, `ART_FILES`). Hereafter is given an excerpt of TELEMAC-2D dictionary regarding the results file:

```
NOM = 'FICHIER DES RESULTATS'
NOM1 = 'RESULTS FILE'
TYPE = CARACTERE
INDEX = 11
MNEMO = `T2D\_FILES\%ADR(T2DRES)'
SUBMIT = 'T2DRES-READWRITE;T2DRES;OBLIG;BIN;ECR;SELAFIN'
DEFAUT = ' '
DEFAUT1 = ' '
```

The character string called SUBMIT is used both by the perl scripts and, through Damocles, by the Fortran programme. It is composed of 6 character strings.
The **first string**, here T2DRES-READWRITE, is made of:

1. the Fortran integer for storing the file number: T2DRES (which is declared in declarations_telemac2d.f)
2. the argument ACTION in the Fortran Open statement that will be used to open the file. ACTION may be READ, WRITE, or READWRITE. Here it is READWRITE because the results file is written, and in case of validation it is read at the end of the computation. It will be stored into T2D_FILES%ADR(T2DRES)%ACTION

The **second string**, here T2DRES, is the name of the file as it will appear in the temporary file where the computation is done.
The **third string** may be OBLIG (the name of the file must always be given), or FACUL (this file is not mandatory).
The **fourth string** (here BIN) says if it is a binary (BIN) or ASCII (ASC) file.
The **fifth string** is just like the READWRITE statement and is used by the perl scripts.
The **sixth string** is also used by the perl scripts and gives information on how the file must be treated. 'SELAFIN' means that the file is a Selafin format, it will have to be decomposed if parallelism is used. Other possibilities are:

SELAFIN-GEOM this is the geometry file

FORTRAN this is the Fortran file for user subroutines

CAS this is the parameter file

CONLIM this is the boundary conditions file

PARAL this file will have an extension added to its name, for distinguishing between processors

DICO this is the dictionary

SCAL this file will be the same for all processors

See Section 15.1 for a more detailed description of the SUBMIT strings.
The following sequence of subroutines is used for opening, using and closing files:
Note : subroutine INIT_FILES2 in BIEF version 5.9 has been renamed BIEF_INIT from version 6.0 on and has from now on nothing to see with files.

1. opening files

```
IFLOT=0
CALL BIEF_OPEN_FILES(CODE,T2D_FILES,44,PATH,NCAR,COUPLAGE,IFLOT,ICODE)
```

   CODE name of calling program in 24 characters

   T2D_FILES the array of BIEF_FILE structures

   44 the size of the previous array

   PATH full name of the path leading to the directory the case is

   NCAR number of characters of the string PATH

   COUPLAGE logical stating if there is a coupling between several programs.

   IFLOT in case of coupling, will be the last logical unit taken by a file

   ICODE code number in a coupling. For example in a coupling between TELEMAC-2D and Sisyphe, TELEMAC-2D will be code 1 and Sisyphe will be code 2.

2. using files

   Most operations on files consist on reading and writing, which always uses the logical unit. Every file has a name in the temporary folder where the program is executed, e.g. T2DRES. The associated file number is an integer with the same name. The logical unit of this file is stored into T2D_FILES(T2DRES)%LU. The logical unit of the geometry file in Sisyphe will be SIS_FILES(SISGEO)%LU.

   Sometimes the real name of files in the original is also used, for example to know if it exists (i.e. has been given in the parameter file). This name is retrieved in the component NAME. For example the name of the geometry file in Sisyphe will be SIS_FILES(SISGEO)%NAME. Note that the name of the same file in the temporary folder is SIS_FILES(SISGEO)%TELNAME. We have in fact:

   ```
   SIS\_FILES(SISGEO)\%TELNAME='SISGEO'.
   ```

3. closing files

   ```
   CALL BIEF\_CLOSE\_FILES(CODE,T2D\_FILES,44,PEXIT)
   ```

   CODE name of calling program in 24 characters

   T2D_FILES the array of BIEF_FILE structures

   44 the size of the previous array

   PEXIT logical, if yes will stop parallelism (in a coupling the last program calling BIEF_CLOSE_FILES will also stop parallelism).

5. Internal structure of BIEF

5.1 BIEF data structure

This chapter will present a description of the finite elements used, the mesh and the storage modes for the finite element matrices.

5.1.1 Description of finite elements

Triangle P1

This is a triangle with linear interpolation. The reference triangle is composed of the coordinate points (0,0) (0,1) and (1,0). On this reference element, the basis functions have the following values :

$P1(\xi,\eta) = 1-\xi-\eta$

$P2(\xi,\eta) = \xi$

$P3(\xi,\eta) = \eta$

Quasi-bubble triangle

The Quasi-Bubble element is obtained by adding an additional point to the three vertices of a triangle. The centre of gravity of the triangle constitutes a natural choice for this fourth point. The initial element P1 is thus divided into three sub-triangles:

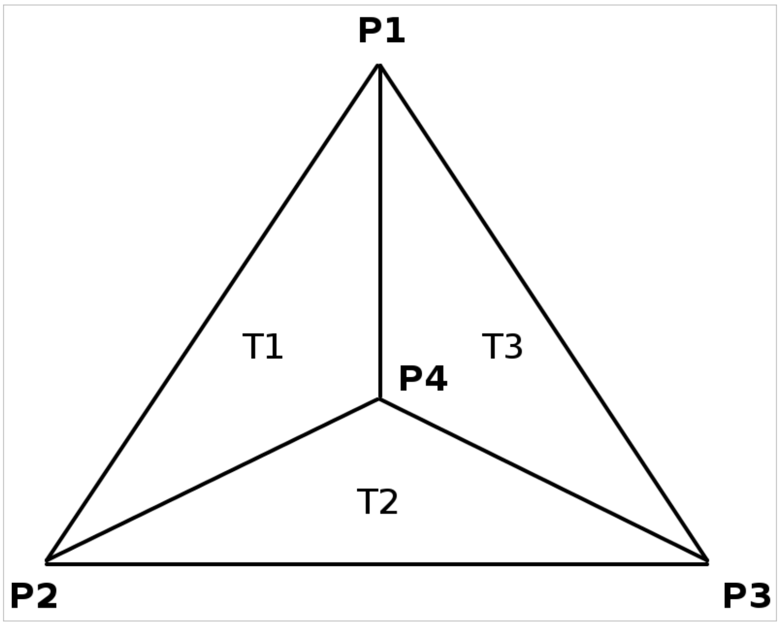


Figure 5.1: Transformation of triangular element T into a quasi-bubble triangle.

By adopting a linear discretisation, the basis functions of the triangle QB (in the sense of finite element) are the 4 Ψ linear functions defined on the triangle T and confirming:

$$\Psi_i(P_j) = \delta_{ij}$$

Quadratic triangle

A quadratic interpolation of the velocity field is a well-known solution to stability problems raised by the Ladyzhenskaya-Babuška-Brezzi condition in Navier–Stokes equations (also called discrete inf-sup condition). The pressure (or the depth in Shallow Water equations) remains linear. For quadratic interpolation, we add 3 degrees of freedom, numbered 4, 5 and 6 on Figure quadratic.

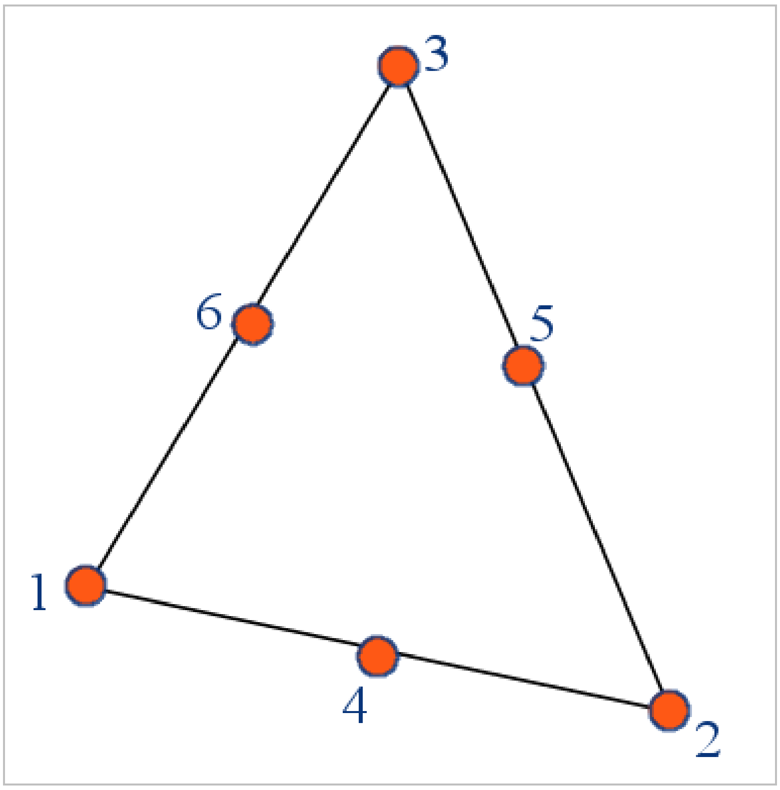


Figure 5.2: quadratic triangle.

The coordinates of the 6 degrees of freedom are:

- Point 1: (0,0)
- Point 2: (1,0)
- Point 3: (0,1)
- Point 4: (1/2,0)
- Point 5: (1/2,1/2)
- Point 6: (0,1/2)

The quadratic interpolation polynoms $P_i(x,y)$, with $i = 1...6$, are such that $P_i(x,y) = \varphi_i(T^{-1}(x,y))$ where T is the isoparametric transformation that gives the real triangle as a function of the reference triangle and φ_i are the basis functions in the reference triangle. In practice T^{-1} is never built and the computation of integrals is done in the reference triangle.
The 6 quadratic basis $\varphi_i(\alpha,\beta)$ are chosen to ensure the following property:

$$\sum_{i=1}^{6} \varphi_i(\alpha,\beta) = 1, \forall(\alpha,\beta) \in triangle$$

Moreover every basis must be equal to 1 on its own point and zero on the five others. This is verified if we take:

$$\text{For } i = 1,2,3,\ \varphi_i(\alpha,\beta) = (2\times\lambda_i(\alpha,\beta) - 1)\times\lambda_i(\alpha,\beta)$$

and for $i = 4,5,6$, $\varphi_i(\alpha,\beta) = 4 \times \lambda_k(\alpha,\beta) \times \lambda_l(\alpha,\beta)$

where k and l are the indices of points of the segment where is point i. More precisely:

$$\varphi_1(\alpha,\beta) = (2 \times \lambda_1(\alpha,\beta) - 1) \times \lambda_1(\alpha,\beta)$$

$$\varphi_2(\alpha,\beta) = (2 \times \lambda_2(\alpha,\beta) - 1) \times \lambda_2(\alpha,\beta)$$

$$\varphi_3(\alpha,\beta) = (2 \times \lambda_3(\alpha,\beta) - 1) \times \lambda_3(\alpha,\beta)$$

$$\varphi_4(\alpha,\beta) = 4 \times \lambda_1(\alpha,\beta) \times \lambda_2(\alpha,\beta)$$

$$\varphi_5(\alpha,\beta) = 4 \times \lambda_2(\alpha,\beta) \times \lambda_3(\alpha,\beta)$$

$$\varphi_6(\alpha,\beta) = 4 \times \lambda_3(\alpha,\beta) \times \lambda_1(\alpha,\beta)$$

Remark: on boundaries a point number 3 is added in the middle and the interpolation polynoms are:

$$\begin{array}{lclcl} \varphi_1(\xi) & = & 2 \times (1-\xi) & \times & (\frac{1}{2} - \xi) \\ \varphi_2(\xi) & = & (2 \times \xi - 1) & \times & \xi \\ \varphi_3(\xi) & = & 4 \times \xi & \times & (1-\xi) \end{array}$$

Quadrilateral Q1

The reference square is comprised of the coordinate points (-1,-1) (1,-1) (1,1) and (-1,1). On this reference element, the base functions have the following values:
$P1(\xi,\eta) = (1 - \xi - \eta + \xi\eta)/4$
$P2(\xi,\eta) = (1 + \xi - \eta - \xi\eta)/4$
$P3(\xi,\eta) = (1 + \xi + \eta + \xi\eta)/4$
$P4(\xi,\eta) = (1 - \xi + \eta - \xi\eta)/4$

Tetrahedron

So far real there is no module in the Telemac system which fully uses this element. In TELEMAC-3D and Estel-3Dmeshes of tetrahedrons are not accepted in.
The reference tetrahedron is comprised of the coordinate points:
(0,0,0) (1,0,0) (0,1,0) (0,0,1). On this reference element, the base functions have the following values:

$$\Psi_1 = (1 - \alpha - \beta - \gamma)$$

$$\Psi_2 = \alpha$$

$$\Psi_3 = \beta$$

$$\Psi_4 = \gamma$$

Prism

This is a prism with 3 vertical rectangular faces, and two triangular faces, one at the bottom and one at the top, and which are not necessarily horizontal.
(The figures indicate local numbering of the nodes).

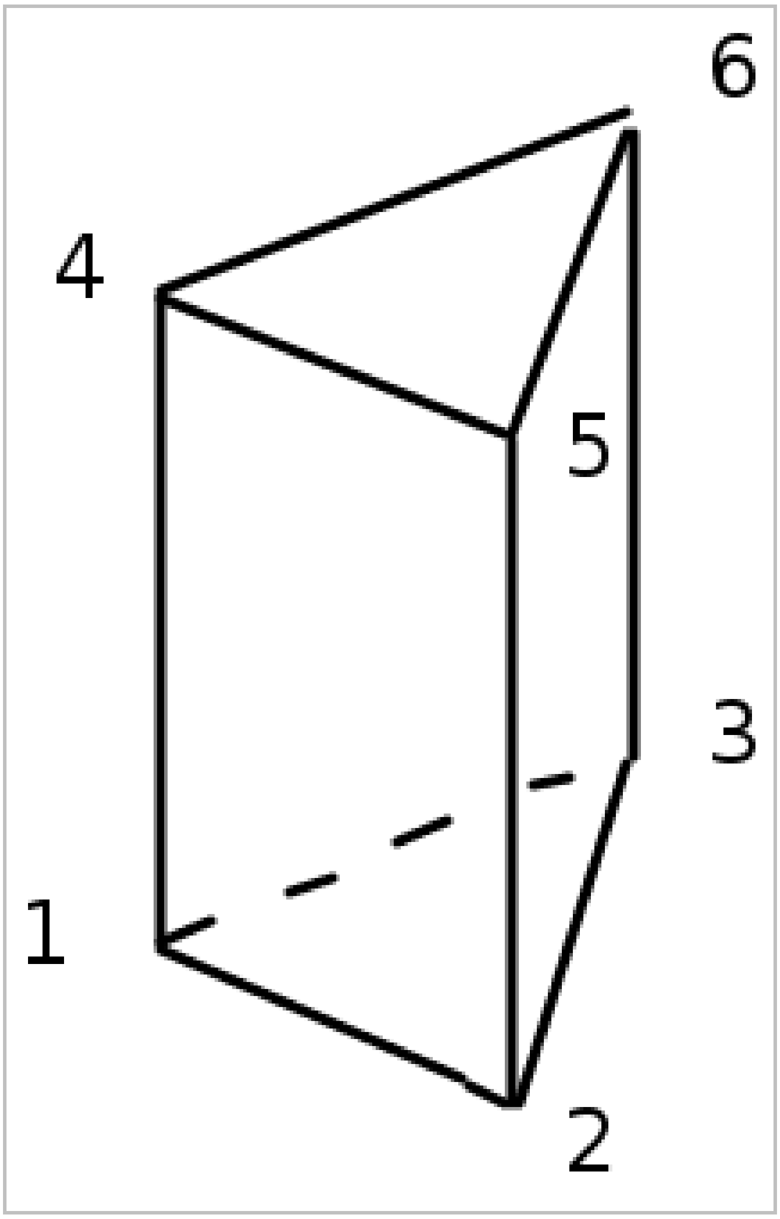


Figure 5.3: Numbering of nodes in a prism

The reference element is as follows:

(the figures in circles indicate local numbering of the nodes).

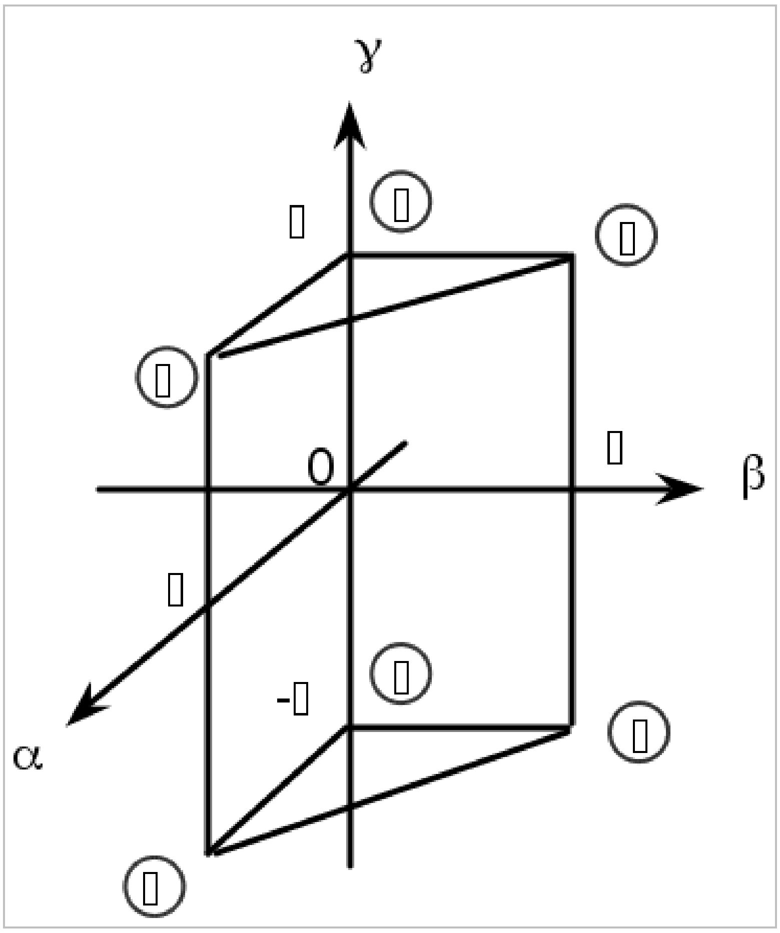


Figure 5.4: Reference element for a prism

The basis functions Ψ_j corresponding to the nodes j of the reference element are:

$$\Psi_1 = (1-\alpha-\beta)\left(\frac{1-\gamma}{2}\right)$$

$$\Psi_2 = \alpha\left(\frac{1-\gamma}{2}\right)$$

$$\Psi_3 = \beta\left(\frac{1-\gamma}{2}\right)$$

$$\Psi_4 = (1-\alpha-\beta)\left(\frac{1+\gamma}{2}\right)$$

$$\Psi_5 = \alpha\left(\frac{1+\gamma}{2}\right)$$

$$\Psi_6 = \beta\left(\frac{1+\gamma}{2}\right)$$

The basis functions ϕ_i on any prism in the ω mesh are obtained by creating the Ψ_i functions with the isoparametric transformation F, transforming the reference prism into this prism of any type.

For a prism in the ω mesh with vertex coordinates (xi,yi,zi), F makes any point M0 with coordinates (α,β,γ) of the reference element correspond to any point M with coordinates (x,y,z) of this prism by:

$$\begin{cases} x = \sum_{i=1}^{6} x_i \Psi_i(\alpha,\beta,\gamma) \\ y = \sum_{i=1}^{6} y_i \Psi_i(\alpha,\beta,\gamma) \\ z = \sum_{i=1}^{6} z_i \Psi_i(\alpha,\beta,\gamma) \end{cases}$$

The Ψ_i functions which appear in the definition of F are the same as the basis functions defined on the reference element since the reference element chosen is isoparametric (the interpolation nodes are also the geometric nodes). In our case, the expressions of F can be simplified since:

```
x1 = x4 ; y1 = y4
x2 = x5 ; y2 = y5
x3 = x6 ; y3 = y6
```

The following is therefore obtained for F :

$$\begin{cases} x = (1-\alpha-\beta)x_1 + \alpha x_2 + \beta x_3 \\ y = (1-\alpha-\beta)y_1 + \alpha y_2 + \beta y_3 \\ z = [(1-\alpha-\beta)z_1 + \alpha z_2 + \beta z_3]\left[\frac{1-\gamma}{2}\right] + [(1-\alpha-\beta)z4 + \alpha z_5 + \beta z_6]\left[\frac{1+\gamma}{2}\right] \end{cases}$$

The following is deduced for the Φ_i functions: $\phi_i(x,y,z) = \Psi_i(F-1(x,y,z))$

5.1.2 Description of mesh

NB: The variables written in capitals are those used in the BIEF FORTRAN program. When a variable is also a component of the BIEF_MESH structure, it is mentioned into commas. For example on the line hereafter (MESH%NELEM) means that NELEM can be retrieved from a BIEF_MESH structure by the component NELEM..

A mesh is composed of NELEM elements (MESH%NELEM) and NPOIN nodes (MESH%NPOIN) known by their coordinates X, Y, Z (respectively MESH%X, Y and Z). Each type of element (triangle P1,prism P0,...) is linked to a code and includes NDP nodes. (MESH%NDP) On an element, the nodes are numbered from 1 to NDP. The connection between this element numbering (local numbering) and the numbering of the mesh nodes from 1 to NPOIN (general numbering) is made through the connectivity table IKLE (MESH%IKLE). The global number of the node with the local number ILOC in the element IELEM is IKLE(IELEM,ILOC).

Table 5.1: Elements in BIEF version 6.2 (the TELEMAC-3D prism is a prism with four vertical quadrangular sides). Quadrilateral elements are kept for an internal use by TELEMAC-3D but no longer maintained.

IELM	NDP(IELM)
00 (segment P0 = constant value)	1
01 (segment P1 = linear)	2
10 (triangle P0 = constant value)	1
11 (triangle P1 = linear)	3
12 (quasi-bubble triangle)	4
13 (quadratic element)	6
20 (quadrilateral Q0 = constant value)	1
21 (quadrilateral Q1 = linear)	4
30 (tetrahedron T0 = constant value	1
31 (tetrahedron T1 = linear	4
40 (prism P0 = constant value)	1
41 (prism P1 = linear)	6
50 (tetrahedron T0 from split prism)	1
51 (tetrahedron T1 from split prism)	4
60 (triangle P0 in a lateral boundary of a mesh of prisms split into tetrahedrons)	1
61 (triangle P1 in a lateral boundary of a mesh of prisms split into tetrahedrons)	3
70 (quadrilateral Q0 in a lateral boundary of a mesh of prisms)	1
71 (quadrilateral Q1 in a lateral boundary of a mesh of prisms)	4
80 (triangle P0 in a boundary of a mesh of tetrahedrons)	1
81 (triangle P1 in a boundary of a mesh of tetrahedrons)	3

In addition, the boundary points of the mesh must be known. These are numbered from 1 to NPTFR (MESH%NPTFR). The connection with the general numbering is made through the table NBOR (MESH%NBOR). NBOR(IPTFR) is the general number of the boundary point IPTFR.

The tables X, Y, Z, IKLE and NBOR are sufficient for defining the mesh. However, it is useful to have other tables available, which can often facilitate the writing of the algorithms. Thus, is it very useful to have tables other than NBOR to describe the boundaries. In fact, three types of numbering can be associated with the boundary of the studied domain. These are the boundary point numbers, the boundary face numbers and the local numbers of the boundary nodes in each of the boundary faces. To connect them, BIEF uses IKLBOR (BIEF%IKLBOR), a connectivity table for the boundary faces, NELBOR (MESH%NELBOR) linking the boundary face numbers to the element numbers to which they belong, and NULONE (MESH%NULONE), a table linking the local numbers of the boundary nodes in the boundary faces to the local numbers of these nodes in the elements to which they belong. The following example illustrates the use of these tables for a triangular element:

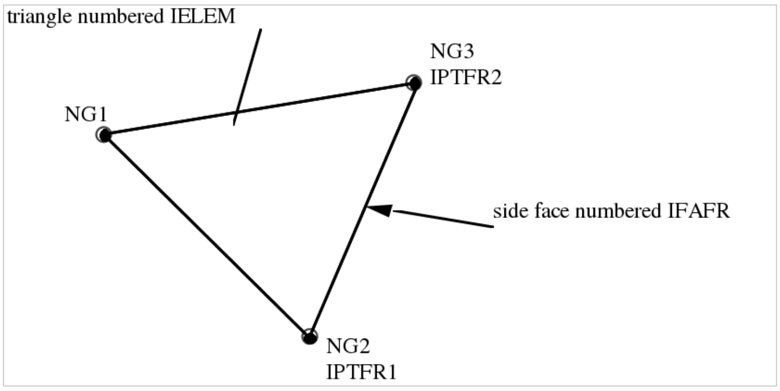


Figure 5.5: numbering of points and faces on boundaries

Take a triangle P1 numbered IELEM constructed on the 3 nodes with global numbers NG1, NG2, NG3. The face defined by the two points NG2 and NG3 is a boundary face with the number IFAFR. The nodes NG2 and NG3 are boundary nodes with the boundary numbers IPTFR1 and IPTFR2. The nodes NG1, NG2 and NG3 have the local numbers 1, 2 and 3 in the triangle. Finally, the nodes IPTFR1 and IPTFR2 have the local numbers 1 and 2 in the boundary face.

We have:

```
   IKLE(IELEM,1) = NG1
   IKLE(IELEM,2) = NG2
   IKLE(IELEM,3) = NG3

   NBOR(IPTFR1) = NG2
   NBOR(IPTFR2) = NG3

   NELBOR(IFAFR) = IELEM

   IKLBOR(IFAFR,1) = IPTFR1
   IKLBOR(IFAFR,2) = IPTFR2

   NULONE(IFAFR,1) = 2
   NULONE(IFAFR,2) = 3
```

For certain elements (prisms), the boundary faces are of two types. Thus, the boundary faces of the prism are triangles or quadrilaterals. A dimension is then added to the tables NELBOR, IKLBOR and NULONE in order to distinguish the type of face in question.

To know the types of boundary faces (segment P1, triangle P1...) for example to calculate boundary matrices, a function IELBOR is used. IELBOR(IELM,1) gives the code of the first type of face of the type IELM element (bottom and top of prisms), IELBOR(IELM,2).gives the type of vertical sides of boundary prisms, which may be triangles or quadrilaterals depending on the fact that the prisms are split into tetrahedrons or not.

The adaptive mesh is simply specified by dimensioning with the maximum possible number of NELMAX elements or the maximum possible number of NELBRX boundary elements all the tables with several dimensions such as IKLE, NULONE...etc.

5.1.3 Storage of matrices

The theoretical aspects of "Element By Element" and “Edge based” storage are discussed below. The resulting conventions are given in appendix 1.

EBE storage

In a finite element code using iterative resolution methods, a matrix is essentially used to multiply it by a vector. Other operations with a matrix are less frequent, and, as will be seen in Chapter IV, these operations can be constructed on the architecture of a matrix-vector product. The storage mode of a matrix has thus been motivated in order to make its vector product as effective as possible.
It is well known that it is not necessary to assemble a finite element matrix to multiply it by a vector. On a mesh of NELEM elements, a matrix M is written as a function of the elementary matrices M_e on each of the elements according to the following:

$$M = \sum_{e=1}^{NELEM} P_e M_e P_e^t$$

where P_e is a transfer matrix between the element and the general mesh. P_e is constructed using the connectivity table. For example, for a triangle P1 with element number IELEM and vertices with general numbers NG1, NG2 and NG3, MIELEM is a matrix 3*3 and PIELEM is a matrix NPOIN*3 such that the coefficient of PIELEM situated at the intersection of row I and column J is 1 if I = IKLE(IELEM,J) and otherwise it is 0.

$$P_{IELEME} = \begin{array}{cl} \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ . & . & . \\ 0 & 1 & 0 \\ . & . & . \\ . & . & . \\ . & . & . \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} & \begin{array}{l} \\ lineIKLE(IELEM,1) \\ \\ lineIKLE(IELEM,2) \\ \\ \\ \\ lineIKLE(IELEM,3) \\ \\ \end{array} \end{array}$$

If X is a vector, the product M.X becomes:$MX = \sum_{e=1}^{NELEM}(P_e M_e P_e^t)X$
which is the same as multiplying M_e by the components of X associated with the nodes of the element e (elementary products), then calculating the sum for all the mesh elements (assembly). It is of course never necessary to construct the matrix P_e which is no other than the connectivity table IKLE.
A matrix M can be stored in the form of NELEM matrices Me. For a mesh of triangles P1, this gives 9*NELEM coefficients. This number can be reduced by retaining only the off-diagonal terms for each elementary matrix and assembling the diagonal terms as shown below.
Let D_e and E_e the diagonal and off-diagonal parts of M_e ($M_e = D_e + E_e$), then:

$$MX = \sum_{e=1}^{NELEM} (P_e D_e P_e^t)X + \sum_{e=1}^{NELEM} (P_e E_e P_e^t)X = DX + \sum_{e=1}^{NELEM} (P_e E_e P_e^t)X$$

where D is the diagonal of M, obtained by assembling the diagonals De.
In BIEF, a matrix MAT is therefore stored in two arrays, one being DMAT, containing the diagonal of the assembled matrix, and the other XMAT, containing the off-diagonal terms of the elementary matrices. For a matrix constructed on a mesh of triangles P1, all that has to be stored is 6*NELEM + NPOIN coefficients, which represents a saving in space of about 2.5*NELEM coefficients compared with complete storage of the element matrices.

In addition, by using elementary matrices, it is possible to obtain a vectorisable matrix vector product on a vector computer. The loop on the elementary products is vectorisable and the assembly loop for these elementary products may also be vectorisable provided a few precautions are taken concerning the numbering of the mesh. We shall look in greater detail at the matrix-vector product and assembly in Chapter IV, which deals with matrix operations.

For storage of off-diagonal elements, the convention adopted in BIEF is as follows. Let us take the case of an element IELEM constructed on NLOC nodes. An elementary matrix Me includes in this case NLOC*(NLOC-1) off-diagonal terms Ei,j, situated in row i and column j of Me.

Let:

```
XMAT(IELEM,1) = E1,2
XMAT(IELEM,2) = E1,3

.........................................

XMAT(IELEM,NLOC-1) = E1,NLOC

.........................................

XMAT(IELEM,NLOC*(NLOC-1)/2) = ENLOC-1,NLOC
```

For the terms in the upper triangular part of Me. If Me is symmetrical, the array XMAT is complete. Otherwise, the lower triangular part of Me must also be stored, which is achieved in the following way:

```

XMAT(IELEM,NLOC*(NLOC-1)/2 + 1) = E2,1

XMAT(IELEM,NLOC*(NLOC-1)/2 + 2) = E3,1

.........................................

XMAT(IELEM,NLOC*(NLOC-1)/2+ NLOC - 1) = ENLOC,1

.........................................

XMAT(IELEM,NLOC*(NLOC-1)) = ENLOC,NLOC-1
```

A matrix MIELEM constructed on a triangle P1 is thus written as a function of XMAT as follows (the * indicate the diagonal terms which are stored elsewhere since they are assembled):

$$M_{IELEM} = \begin{pmatrix} * & XMAT(IELEM,1) & XMAT(IELEM,2) \\ XMAT(IELEM,4) & * & XMAT(IELEM,3) \\ XMAT(IELEM,5) & XMAT(IELEM,6) & * \end{pmatrix}$$

The following table summarises, for a few types of elements, the memory space required for storing a matrix (for reference purposes, the space needed for compact storage is indicated).

Type of element	BIEF storage	Compact storage
Quadrilateral Q1	NPOIN+12 NELEM=13 NPOIN	19 NPOIN
Triangle P1	NPOIN+ 6 NELEM=13 NPOIN	15 NPOIN
Triangle P2	NPOIN+30 NELEM=16 NPOIN	24 NPOIN
Quadrilateral Q2 (9 nodes)	NPOIN+72 NELEM=19 NPOIN	33 NPOIN
Brick P1	NPOIN+56 NELEM=57 NPOIN	55 NPOIN
Prism TELEMAC-3D	NPOIN+30 NELEM=61 NPOIN	43 NPOIN

EDGE-BASED storage

Edge-based storage is a recent technique which enables to store a matrix in an optimal and easy way. The idea is that the element of the matrix, let's say e.g. $\int_\Omega \Psi_i \Psi_j d\Omega$, with i different from j, is not equal to 0 only if points I and j are linked by a segment of the mesh. Every segment is thus the best location to store these off-diagonal terms. For a non symmetrical matrix, there will be two coefficients to store on every segment, for a symmetrical matrix, only one will be necessary. This can be extended to complex elements such as quasi-bubble by adding the relevant segments. The data structure to deal with such a storage is very simple:

An array called GLOSEG, equivalent of IKLE for elements, which gives the global numbers of the two ends of the segment. Its dimension in Fortran is (NSEG,2) where NSEG is the total number of segments, i.e. for triangles : (3*NELEM+NPTFR)/2.

An array called ELTSEG, with dimensions (NELEM,NS), where NS is the number of segments in an element.(3 for a triangle). ELTSEG gives for every element the segment numbers of its 3 segments.

An array ORISEG, with dimensions (NELEM,NS). ORISEG gives the orientation of every segment in an element, i.e. it is equal to 1 if the segment is in counter-clockwise orientation (from its point 1 to its point 2), and is equal to 2 otherwise.

A matrix storage then consists of:

- A diagonal
- Two arrays XA1 and XA2 of size NSEG.

XA1 contains the coefficient of point 2 in equation of point 1, and XA2 its symmetrical part, coefficient of point 1 in equation of point 2.

XA2 is not necessary if the matrix is symmetrical. When the matrix is rectangular, XA2 first contains the part symmetrical to XA1, then the extra terms, each one corresponding with a segment and with the same order as the segments.

The matrix thus stored is assembled.

The local numbering of segments in an element is the following:

Linear triangle:

Segment 1 goes from point 1 to point 2 or from point 2 to point 1 (depending of ORISEG) Segment 2 goes from point 2 to point 3 or from point 3 to point 2 (depending of ORISEG) Segment 3 goes from point 3 to point 1 or from point 1 to point 3 (depending of ORISEG)

Quasi-bubble triangle:

Segment 1 goes from point 1 to point 2 or from point 2 to point 1 (depending of ORISEG) Segment 2 goes from point 2 to point 3 or from point 3 to point 2 (depending of ORISEG) Segment 3 goes from point 3 to point 1 or from point 1 to point 3 (depending of ORISEG) Segment 4 goes from point 1 to point 4 Segment 5 goes from point 2 to point 4 Segment 6 goes from point 3 to point 4

Segments 4 to 6 need no value of ORISEG, they always go from a linear point to the quadratic point. This is used in matrix-vector products algorithms, see subroutine MVSEG.

Quadratic triangle:

Segment 1 goes from point 1 to point 2 or from point 2 to point 1 (depending of ORISEG) Segment 2 goes from point 2 to point 3 or from point 3 to point 2 (depending of ORISEG) Segment 3 goes from point 3 to point 1 or from point 1 to point 3 (depending of ORISEG) Segment 4 goes from point 1 to point 4 Segment 5 goes from point 2 to point 5 Segment 6 goes from point 3 to point 6 Segment 7 goes from point 2 to point 4 Segment 8 goes from point 3 to point 5 Segment 9 goes from point 1 to point 6 Segment 10 goes from point 1 to point 5 Segment 11 goes from point 2 to point 6 Segment 12 goes from point 3 to point 4 Segment 13 goes from point 4 to point 5 Segment 14 goes from point 5 to point 6 Segment 15 goes from point 6 to point 4

ORISEG is not useful for segments 4 to 15. For segments 4 to 12 the principle is that the first point is linear (1, 2 or 3) and the second is quadratic (4, 5 or 6). Note that in rectangular linear-quadratic matrices, segments 13, 14 and 15 will not appear as they link only quadratic points. This is why they have been put at the end, so that we have no gap in segment numbering for rectangular matrices.

The total number of segments 4 to 6 is NSEG.

The total number of segments 7 to 9 is NSEG.

The total number of segments 10 to 11 is 3 NELEM

The total number of segments 13 to 15 is 3 NELEM

Quadratic boundary segments have also a local numbering. Point 1 and point 2 are defined as in lilnear segments, point 3 is in the middle.

Linear prism:

Horizontal segments:

Segment 1 goes from point 1 to point 2 or from point 2 to point 1 (depending of ORISEG)
Segment 2 goes from point 2 to point 3 or from point 3 to point 2 (depending of ORISEG)
Segment 3 goes from point 3 to point 1 or from point 1 to point 3 (depending of ORISEG)
Segment 4 goes from point 4 to point 5 or from point 5 to point 4 (depending of ORISEG)
Segment 5 goes from point 5 to point 6 or from point 6 to point 5 (depending of ORISEG)
Segment 6 goes from point 6 to point 4 or from point 4 to point 6 (depending of ORISEG)

Vertical segments:

Segment 7 goes from point 1 to point 4 Segment 8 goes from point 2 to point 5 Segment 9 goes from point 3 to point 6

Crossed segments (for their global numbering see subroutine STOSEG41):

Segment 10 goes from point 1 to point 5 Segment 11 goes from point 2 to point 4 Segment 12 goes from point 2 to point 6 Segment 13 goes from point 3 to point 5 Segment 14 goes from point 3 to point 4 Segment 15 goes from point 1 to point 6

5.2 Construction of matrices

The BIEF matrices are calculated exactly through analytical integration. The terms of a finite element matrix are generally polynomial integrals, which can be estimated through successful completion of the analytical integration. On paper, the analytical integration is long, tedious and a source of error, even though it is possible to take a few short cuts. This is why we prefer the formal calculation software programme MAPLE V, which can give in FORTRAN the exact result of an integral calculation.

An example is given below of a matrix calculation as it can be carried out with MAPLE V. The full description is given in the reference J.-M. and LENORMANT [3].

5.2.1 Example of a mass-matrix calculation

As an example, we choose here to calculate the mass matrix on a mesh of quadrilaterals Q1. It is a little more complicated than linear triangles, but will show that the Jacobian of isoparametric transformations is not always a constant.

It is sufficient to conduct the calculation on a quadrangle Q with vertices P1, P2, P3, P4 with coordinates (x1,y1), (x2,y2), (x3,y3) and (x4,y4). The element Mi,j of the elementary mass matrix is written as follows:$M_{i,j} = \int_Q \Psi_i \Psi_j dQ$.

where Ψ_i is the base function associated with the node i (i=1,2,3 or 4).

We thus calculate the integral on a reference element thanks to an isoparametric transform T. Any point of the reference element Q0 with coordinates (ξ,η) is associated with a point on the quadrilateral Q with coordinates (x,y) such that: $\begin{cases} x(\xi,\eta) = t_1 + t_2\xi + t_3\eta + t_4\xi\eta \\ y(\xi,\eta) = t'_1 + t'_2\xi + t'_3\eta + t'_4\xi\eta \end{cases}$

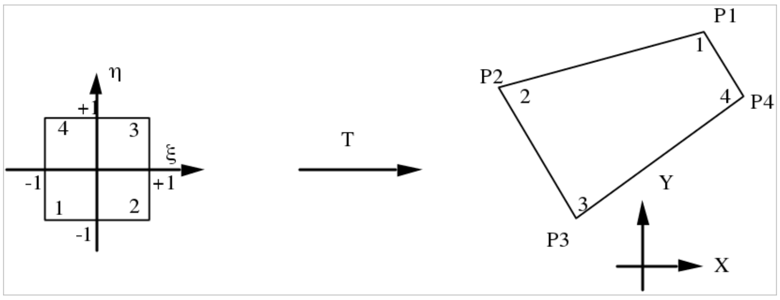


Figure 5.6: Isoparametric transformation (the numbers in the quadrilaterals indicate local numbering)

The image by T of each vertex of the reference element thus gives a vertex of the quadrilateral, which, by identification, provides the coefficients t1, t2, ... of the transformation, as a function of the coordinates x1,y1 x2,y2 x3,y3 x4,y4 of the vertices:
$t_1 = (+x1 + x2 + x3 + x4)/4$
$t_2 = (-x1 + x2 + x3 - x4)/4$
$t_3 = (-x1 - x2 + x3 + x4)/4$
$t_4 = (+x1 - x2 + x3 - x4)/4$
$t'_1 = (+y1 + y2 + y3 + y4)/4$
$t'_2 = (-y1 + y2 + y3 - y4)/4$
$t'_3 = (-y1 - y2 + y3 + y4)/4$
$t'_4 = (+y1 - y2 + y3 - y4)/4$
A base Ψ in the real element corresponds in the reference element to a polynomial P such that $\Psi(x,y) = T(P(\xi,\eta))$.
In our case, there are 4 polynomials associated with the 4 bases of the real element:
$P1(\xi,\eta) = (1 - \xi - \eta + \xi\eta)/4$
$P2(\xi,\eta) = (1 + \xi - \eta - \xi\eta)/4$
$P3(\xi,\eta) = (1 + \xi + \eta + \xi\eta)/4$
$P4(\xi,\eta) = (1 - \xi + \eta - \xi\eta)/4$
As for the bases Φ, each polynomial has a value of 1 for one vertex of the element and 0 for the others.
In the reference element, the integral being sought takes the value:

$$\int_Q \Psi_i \Psi_j dQ = \int_{-1}^{+1} \int_{-1}^{+1} P_i P_j \,|J|\, d\xi d\eta$$

where J is the Jacobian of the transformation T , equal to the determinant of the Jacobian matrix:

$$\begin{matrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} \end{matrix}$$

Let:
$J = (t_2 + t_4\eta)(t'_3 + t'_4\xi) - (t'_2 + t'_4\eta)(t_2 + t_4\xi)$

J is assumed to be positive, which is obtained with local numbering of the points which run along the boundary of the element in the counter-clockwise sense. J is not constant (it is with linear triangles).
Since J is a polynomial, then we have the integral of a polynomial (of which the term with the highest degree is in $\xi_3\eta_3$).
This information is sufficient for MAPLE V to successfully carry out the calculation. For example, for this calculation of a mass matrix, the following can be obtained:

```
!FORMAL CALCULATION OF A Q1 MASS MATRIX :

      MAT(1,1)=(X2*(2.*Y4+Y3)+X3*(Y4-Y2)+X4*(-Y3-2.*Y2))/36.
      MAT(1,2)=(X2*(Y4+2.*Y3)+X3*(Y4-2.*Y2)-X4*(Y3+Y2))/72.
      MAT(1,3)=(X2*Y3+X3*(Y4-Y2)-X4*Y3)/72.
      MAT(1,4)=(X2*(Y4+Y3)+X3*(2.*Y4-Y2)+X4*(-2.*Y3-Y2))/72.
      MAT(2,1)=(X2*(Y4+2.*Y3)+X3*(Y4-2.*Y2)-X4*(Y3+Y2))/72.
      MAT(2,2)=(3.*X2*Y3+X3*(Y4-3.*Y2)-X4*Y3)/36.
      MAT(2,3)=(X2*(-Y4+3.*Y3)+X3*(2.*Y4-3.*Y2)+X4*(-2.*Y3+Y2))/72.
      MAT(2,4)=(X2*Y3+X3*(Y4-Y2)-X4*Y3)/72.
      MAT(3,1)=(X2*Y3+X3*(Y4-Y2)-X4*Y3)/72.
      MAT(3,2)=(X2*(-Y4+3.*Y3)+X3*(2.*Y4-3.*Y2)+X4*(-2.*Y3+Y2))/72.
      MAT(3,3)=(X2*(-2.*Y4+3.*Y3)+3.*X3*(Y4-Y2)+X4*(-3.*Y3+2.*Y2 ))/36.
      MAT(3,4)=(X2*(-Y4+2.*Y3)+X3*(3.*Y4-2.*Y2)+X4*(-3.*Y3+Y2))/72.
      MAT(4,1)=(X2*(Y4+Y3)+X3*(2.*Y4-Y2)+X4*(-2.*Y3-Y2))/72.
      MAT(4,2)=(X2*Y3+X3*(Y4-Y2)-X4*Y3)/72.
      MAT(4,3)=(X2*(-Y4+2.*Y3)+X3*(3.*Y4-2.*Y2)+X4*(-3.*Y3+Y2))/ 72.
      MAT(4,4)=(X2*Y3+X3*(3.*Y4-Y2)-3.*X4*Y3)/36.
```

On a vector computer, the previous FORTRAN expressions, integrated in a loop on the elements, are vectorised.
The above demonstration can also be conducted in the same way with any matrix which gives the integral of a polynomial expression. This is the case of mass matrices, divergence type matrices. For diffusion matrices, it is the case with linear triangles, not with quadrilaterals.

5.2.2 Matrices with a quasi-bubble element

The matrices to be calculated are of the type:

$$M(i,j) = \int_{\Omega} f(\Psi_j, \varphi_i, F, G, H, U, V, W) d\Omega$$

In these matrices, the test functions φ and the basis functions Ψ could be of two different types (P1 or Quasi-Bubble), as well as the discretisation functions of the variables F,U,V...
Three cases are possible:
<u>a - φ and Ψ are of type P1:</u>
This is the standard case. The elementary matrices are then composed of 9 terms and their calculation is carried out by integration on a reference element by using a transformation called isoparametric transformation.
<u>b - φ and Ψ are Quasi-Bubble type:</u>
Elementary matrices of this type have 16 terms. These terms are calculated easily on the basis of the calculation of the terms P1 thanks to the dividing up of the triangle T into three sub-triangles.
In fact, what we have is:

$$M(i,j) = \underbrace{\int_{T1} f(\Psi_j^{T1}, \varphi_i^{T1}, F, ...) d\Omega}_{\text{I1}} + \underbrace{\int_{T2} f(\Psi_j^{T2}, \varphi_i^{T2}, F, ...) d\Omega}_{\text{I2}} + \underbrace{\int_{T3} f(\Psi_j^{T3}, \varphi_i^{T3}, F, ...) d\Omega}_{\text{I3}}$$

where the power indices denote the restrictions of the functions on the triangles in question. The restrictions of the basis function of the Quasi-Bubble element to the sub-triangles are the basis functions P1 on these sub-triangles. Calculation of each of the integrals I1, I2, and I3 is thus obtained independently by the method described in a. The sum of these integrals must then be determined. In addition, the intersection of the supports of the Quasi-Bubble basis functions is only made rarely on the three sub-triangles and often on a single sub-triangle (off-diagonal terms). This results in the deletion of one or two of the integrals I1, I2, and I3.

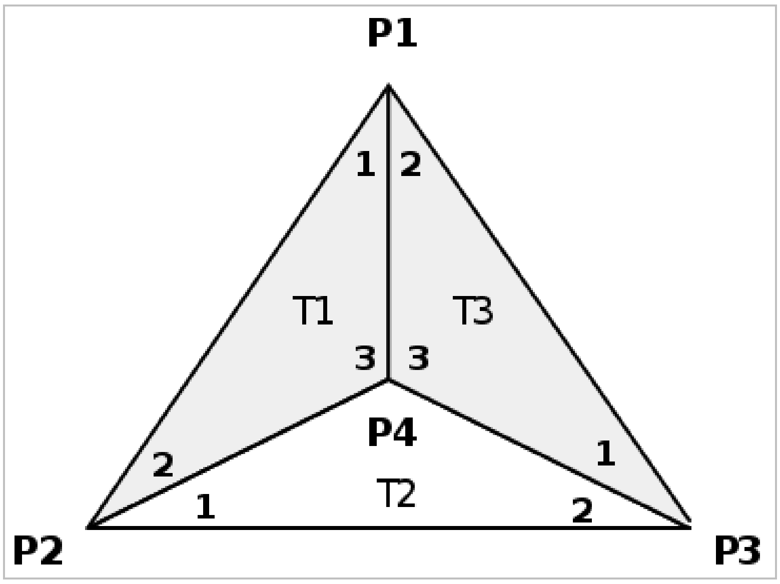


Figure 5.7: Support of quasi-bubble function Ψ_1 (shaded) and local numbering within the sub-triangles.

It can thus be observed that only the function Ψ_4 has a support which coincides with the triangle T.
e.g.: calculation of the term $M_{1,1}$:
we have:

$$\begin{array}{lcccccc} M_{1,1} & = & \int_{T1} f(\Psi_1^{T1}, \varphi_1^{T1}, F, ...) d\Omega & + & 0 & + & \int_{T3} f(\Psi_1^{T3}, \varphi_1^{T3}, F, ...) d\Omega \\ & = & m1_{1,1} & + & 0 & + & m3_{2,2} \end{array}$$

m1, m2, or m3 designating the matrix P1 calculated on the sub-triangle Pi. In fact, is the base function assigned to the first point of the sub-triangle T1, and is the basis function assigned to the second point of the sub-triangle T3.
The matrix M Quasi-Bubble x Quasi-Bubble is thus finally obtained thanks to pre-assembling of sub-matrices P1. All these operations are summarised in the following table: $M_{1,1} = m1_{1,1} + m3_{2,2}$
$M_{1,2} = m1_{1,2}$
$M_{1,3} = m3_{2,1}$
$M_{1,4} = m1_{1,3} + m3_{2,3}$
$M_{2,1} = m1_{2,1}$
$M_{2,2} = m1_{2,2} + m2_{1,1}$
$M_{2,3} = m2_{1,2}$
$M_{2,4} = m1_{2,3} + m2_{1,3}$
$M_{3,1} = m3_{1,2}$

$M_{3,2} = m2_{2,1}$

$M_{3,3} = m2_{2,2} + m3_{1,1}$

$M_{3,4} = m2_{2,3} + m3_{1,3}$

$M_{4,1} = m1_{3,1} + m3_{3,2}$

$M_{4,2} = m1_{3,2} + m2_{3,1}$

$M_{4,3} = m2_{3,2} + m3_{3,1}$

$M_{4,4} = m1_{3,3} + m2_{3,3} + m3_{3,3}$

c - φ and Ψ are of different types:

The elementary matrices of this type are rectangular and include 12 terms. Here, we shall deal with the case where φ is P1 and Ψ Quasi-Bubble; the symmetrical situation results directly from this.

The following can still be written:

$$M(i,j) \quad = \quad \underset{I1}{\int_{T1} f(\Psi_j^{T1}, \varphi_i^{T1}, F, ...)d\Omega} \quad + \quad \underset{I2}{\int_{T2} f(\Psi_j^{T2}, \varphi_i^{T2}, F, ...)d\Omega} \quad + \quad \underset{I3}{\int_{T3} f(\Psi_j^{T3}, \varphi_i^{T3}, F, ...)d\Omega}$$

Unlike the situation encountered in b), the restrictions of the functions φ to the sub-triangles no longer correspond to the base functions P1 on these sub-triangles. In fact, what we have is:

$\varphi_i(P_j) = \sigma_{ij} for 1 \leq j \leq 3$

and:

$\varphi_i(P_4) = \frac{1}{3}$

since P_4 is the centre of gravity of the triangle T.

In the internal numbering of the sub-triangles Ti , P_4 always corresponds to the point n°3, so that we have the following basis functions in the reference triangle:

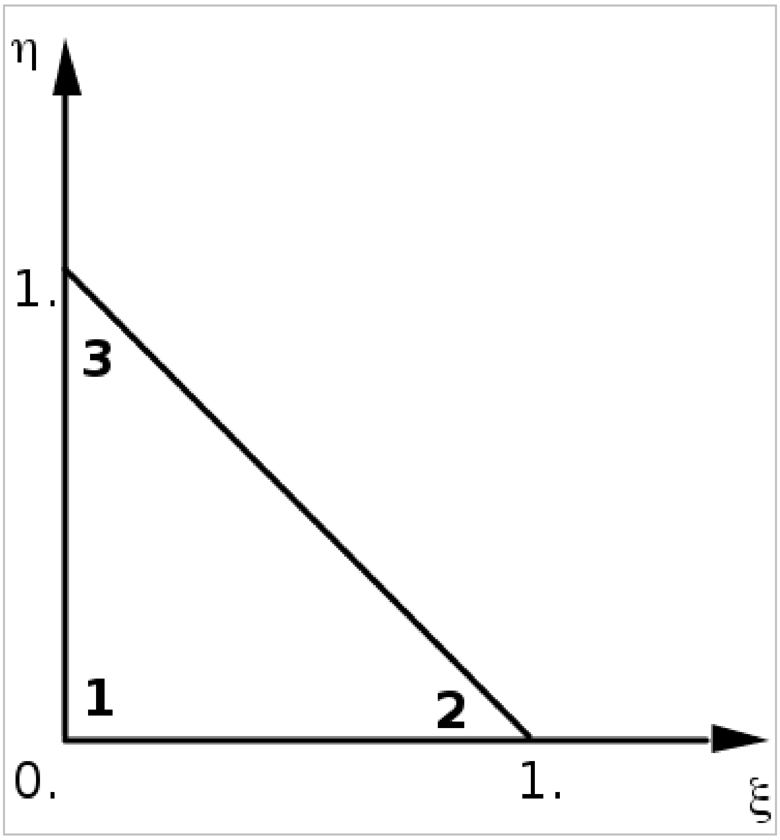


Figure 5.8: Reference element for a triangle

function P	P(1)	P(2)	P(3)
$P_1(\xi,\eta) = 1-\xi-\frac{2}{3}\eta$	1	0	$\frac{1}{3}$
$P_2(\xi,\eta) = \xi+\frac{1}{3}\eta$	1	0	$\frac{1}{3}$
$P_3(\xi,\eta) = \frac{1}{3}\eta$	1	0	$\frac{1}{3}$

The isoparametric transformation retains the value of the functions at the nodes, so that the anticipated result is obtained in the real mesh.
The matrix coefficients on the triangle T are obtained by assembling on the sub-triangles:
$M_{1,1} = m1_{1,1} + m3_{2,2}$
$M_{1,2} = m1_{1,2} + m2_{3,1}$
$M_{1,3} = m2_{3,2} + m3_{2,1}$
$M_{1,4} = m1_{1,3} + m2_{3,3} + m3_{2,3}$
$M_{2,1} = m1_{1,2} + m3_{3,2}$
$M_{2,2} = m1_{2,2} + m2_{1,1}$
$M_{2,3} = m2_{1,2} + m3_{3,1}$
$M_{2,4} = m1_{2,3} + m2_{1,3} + m3_{3,3}$
$M_{3,1} = m1_{3,1} + m3_{1,2}$
$M_{3,2} = m1_{3,2} + m2_{2,1}$
$M_{3,3} = m2_{2,2} + m3_{1,1}$
$M_{3,4} = m1_{3,3} + m2_{2,3} + m3_{1,3}$
In the opposite case of a Quasi-Bubble*P1 matrix, the following would be obtained:
$M_{1,1} = m1_{1,1} + m3_{2,2}$
$M_{1,2} = m1_{1,2} + m3_{2,3}$
$M_{1,3} = m1_{1,3} + m3_{2,1}$

$M_{2,1} = m1_{2,1} + m2_{1,3}$
$M_{2,2} = m1_{2,2} + m2_{1,1}$
$M_{2,3} = m1_{2,3} + m2_{1,2}$
$M_{3,1} = m2_{2,3} + m3_{1,2}$
$M_{3,2} = m2_{2,1} + m3_{1,3}$
$M_{3,3} = m2_{2,2} + m3_{1,2}$
$M_{4,1} = m1_{3,1} + m2_{3,3} + m3_{3,2}$
$M_{4,2} = m1_{3,2} + m2_{3,1} + m3_{3,3}$
$M_{4,3} = m1_{3,3} + m2_{3,2} + m3_{3,1}$

5.3 Matrix operations:

It was shown above that matrix operations in BIEF are carried out at elementary level first of all and then assembled.
This section gives a detailed description of the assembly algorithm and the main matrix operations carried out in BIEF, in the case of an element by element storage, namely:

- Product of a non symmetrical matrix and a vector
- Product of a symmetrical matrix and a vector
- Product of the transpose of a matrix and a vector
- Processing of Dirichlet-type boundary conditions in the matrices
- Diagonal preconditioning

The main algorithm is in fact the product of a matrix and a vector, as it will be seen that all the others can be reduced to this, or at least be derived from it.
Then in the last section we shall detail the matrix-vector product when using an edge-based storage.

5.3.1 Assembly of an elementary vector

With a known vector We of dimension NLOC for each element, a general vector R of dimension NPOIN must be defined. Using the notation of chapter I, this is written as follows:

$$R = \sum_{e=1}^{NELEM} (P_e W_e)$$

Taking the example of the triangle P1, if the components of the vector WIELEM are designated W1, W2, and W3 , then W1(IELEM) is the vector component at the node with local number 1 of element IELEM, etc.
In FORTRAN, R is defined as follows:

```
DO IELEM=1,NELEM
  R(IKLE(IELEM,1)) = R(IKLE(IELEM,1))  +  W1(IELEM)
  R(IKLE(IELEM,2)) = R(IKLE(IELEM,2))  +  W2(IELEM)
  R(IKLE(IELEM,3)) = R(IKLE(IELEM,3))  +  W3(IELEM)
ENDDO
```

where IKLE is the connectivity table: IKLE(IELEM,I) is the general number of the Ith local node of element IELEM.
This loop can be vectorised, as will be seen below.
The assembly loop is first of all transformed into three successive loops:

```
!
DO IELEM=1,NELEM
  R(IKLE(IELEM,1))=R(IKLE(IELEM,1))+W1(IELEM)
ENDDO
!
DO IELEM=1,NELEM
  R(IKLE(IELEM,2))=R(IKLE(IELEM,2))+W2(IELEM)
ENDDO
!
DO IELEM=1,NELEM
  R(IKLE(IELEM,3))=R(IKLE(IELEM,3))+W3(IELEM)
ENDDO
```

These three loops are not automatically vectorised on a vector computer. Indeed, the principle of vectorisation is to work in real time on a number of elements of the loop. This number, referred to as the vector length of the computer, varies from one supercomputer to another. It is 64 or 128 on a Cray YMP and up to 1024 on a Fujitsu. Taking the Cray as an example, a loop running from 1 to NELEM will be processed in 64-element clusters. Thus, if loop 1 is vectorised on a Cray computer, the instruction R(IKLE(IELEM,1))= R(IKLE(IELEM,1)) +W1(IELEM) will be executed simultaneously for elements 1 to 64, 65 to 128 and so on. It is clear, therefore, that the result can only be correct if each component of vector R is used only once in each cluster of 64 elements, i.e. if there are not two elements IELEM1 and IELEM2 in the same cluster such that IKLE(IELEM1,1)=IKLE(IELEM2,1). During compilation, the Cray will detect any problem of backward dependency and not vectorise the loop.

It is, however, possible to force vectorisation, but in this case it is essential to ensure that the grid does not contain any backward dependencies. This again shows the advantages of having split the initial assembly loop into three, as otherwise the condition of non-dependency would have been more severe and hence more difficult to achieve. It would have been necessary for IKLE(IELEM1,I) – IKLE(IELEM2,J) for I,J = 1,2,3 for all different elements IELEM1, IELEM2 contained in each 64-element batch.

With a split assembly loop on the Cray, backward dependencies occurs if 2 different elements IELEM1 and IELEM2 are such that:

```
IELEM1/64 = IELEM2/64  !(/ here indicates the complete division)
```

and if I=1,2, or 3 such that

```
IKLE(IELEM1,I) = IKLE(IELEM2,I)
```

On a Fujitsu computer or similar, 64 must be replaced by 1024. The set conditions for the grid are thus more severe.

In order to vectorise the three loops, it is necessary to find a system for numbering the elements that eliminates any backward dependencies. This leads to a paradoxical situation as such a numbering system is impossible in theory yet easy to apply in practice. Indeed:

- there are counter-examples if the number of elements is too small,
- heuristic algorithms easily find a large number of acceptable numbering systems if the number of elements is sufficient (in practice sufficiently larger than the vector length, i.e. 64 for a Cray).

A counter-example and then a "heuristic" algorithm will therefore be discussed below.

Counter-example:

It is sufficient to consider a grid of triangles containing less than 64 elements, in which one point belongs to four different triangles. This point must have the same local number (1, 2 or 3) in at least two of these triangles, which will create a backward dependencies that is impossible to eliminate.

Element numbering algorithm

The basic idea is to search for dependency situations and progressively eliminate them. Starting with an existing system (for more than 64 elements), the algorithm goes through the numbering and examines all sequences of 64 elements. When a faulty element appears, its number is exchanged with that of a higher-ranking element.

The algorithm fails if there are still dependencies and no higher ranking element. In this case the numbers are exchanged with those of a lower-ranking element, which means that the previous checks are invalidated. The entire algorithm is therefore rerun!

In practice, this algorithm is extremely efficient and rarely has to be run more than twice. This is due to the fact that, as soon as there are more than several hundred elements, the combinational provides a large number of suitable numbering systems.

Once the elements have been numbered, it is simply a question of informing the compiler that there are no backward dependencies in the loops that it will encounter (command CDIR$ IVDEP on a Cray, *VOCL LOOP,NVREC on Siemens-Fujitsu).

In the case of a large vector length, there is no guarantee that a solution will exist for average grids (containing a few thousand elements). In order to benefit from vectorisation, however, it is still possible to split the assembly loops into sub-loops involving only batches of elements that contain no backward dependencies. In this case, vectorisation is forced for all these sub-loops.

Assuming that the following loop is valid for a vector length of 64:

```
!
        DO IELEM=1,NELEM
            R(IKLE(IELEM,1))=R(IKLE(IELEM,1))+W1(IELEM)
        ENDDO
!
```

it can be transposed for higher vector-lengths as follows:

```
!
       M64 = NELEM/64
       N64 = MOD(NELEM,64)
!
       DO K =1,M64
         DO IELEM=(K-1)*64+1,K*64
           R(IKLE(IELEM,1))=R(IKLE(IELEM,1))+W1(IELEM)
         ENDDO
       ENDDO
!
       DO IELEM=M64*64+1,M64*64+N64
         R(IKLE(IELEM,1))=R(IKLE(IELEM,1))+W1(IELEM)
       ENDDO
!
```

Vectorisation of loops 2 and 3 may be forced.

Tests on a Cray YMP show that vectorisation provides very considerable savings in the amount of time required for vector assembly:

- factor of 19 for quadrilaterals with bilinear interpolation (4 loops),
- factor of 12 for triangles with linear interpolation (3 loops).

As vector assembly operations are used intensively in the algorithms, the overall amount of time saved is also appreciable (up to a factor of 3).

5.3.2 Product non symmetrical matrix by vector

The problem involves calculating the vector R, which is the product of the matrix M and the vector V. It will be recalled that:

$$R = MV = DV + \sum_{e=1}^{NELEM} (P_e E_e P_e^t).V$$

The example of quadrilaterals Q1 is discussed below. The matrix M is stored in the form of two arrays DM(NPOIN) and XM(NELEM,12).
The FORTRAN instructions are as follows:
Contribution of the diagonal: product of D and V (loop that can be expressed in vector form):

```
DO I=1,NPOIN
  R(I) = DM(I) * V(I)
ENDDO
```

Contribution of off-diagonal terms: products $E_e(P_e^t V)$ stored in working arrays W1, W2, W3 and W4. This loop can also be expressed in vector form.

```
DO IELEM=1,NELEM
```

General numbers of points for the element (given by the array IKLE)

```
  I1 = IKLE(IELEM,1)
  I2 = IKLE(IELEM,2)
  I3 = IKLE(IELEM,3)
  I4 = IKLE(IELEM,4)
```

As far as the element is concerned, the results concerning points with different local numbers are stored separately (for numbers 1: W1, etc.)

```
  W1(IELEM) = + XM(IELEM, 1) * V(I2)
              + XM(IELEM, 2) * V(I3)
              + XM(IELEM, 3) * V(I4)

  W2(IELEM) = + XM(IELEM, 7) * V(I1)
              + XM(IELEM, 4) * V(I3)
              + XM(IELEM, 5) * V(I4)

  W3(IELEM) = + XM(IELEM, 8) * V(I1)
              + XM(IELEM,10) * V(I2)
              + XM(IELEM, 6) * V(I4)

  W4(IELEM) = + XM(IELEM, 9) * V(I1)
              + XM(IELEM,11) * V(I2)
              + XM(IELEM,12) * V(I3)

ENDDO
```

The vector defined by W1, W2, W3 and W4 is assembled and then added to R, which already contains the contribution of the diagonal.
This algorithm is very easy to explain. Taking as an example the term XM(IELEM,1), this is conventionally the term MAT(1,2) for element IELEM. It is thus a part of the coefficient of point 2 of element IELEM in the equation for point 1 of the same element. The product XM(IELEM,1)*V(I2) must therefore be added to the result R(I1). This is what happens in loop 2 and the assembly loop via working array W1.
To summarise the method, it may be said that the vectors, and no longer the matrices, are assembled. In a method involving classical compacting, vectorisation of the product matrix x vector is broken by an internal loop on the surrounding points.

5.3.3 Product symmetrical matrix by vector

When the matrix is symmetrical, the terms XM(IELEM,NLOC*(NLOC-1)/2+1) to XM(IELEM,NLOC*(NLOC-1)) are no longer stored as they are equal respectively to XM(IELEM,1),...,XM(IELEM,NLOC*(NLOC-1)/2).

In calculating the working arrays W1,... , they simply need to be substituted, so that the following are obtained, still for quadrilaterals Q1:

```
W1(IELEM) = + XM(IELEM,1) * V(I2)
            + XM(IELEM,2) * V(I3)
            + XM(IELEM,3) * V(I4)

W2(IELEM) = + XM(IELEM,1) * V(I1)
            + XM(IELEM,4) * V(I3)
            + XM(IELEM,5) * V(I4)

W3(IELEM) = + XM(IELEM,2) * V(I1)
            + XM(IELEM,4) * V(I2)
            + XM(IELEM,6) * V(I4)

W4(IELEM) = + XM(IELEM,3) * V(I1)
            + XM(IELEM,5) * V(I2)
            + XM(IELEM,6) * V(I3)
```

5.3.4 Product transposed matrix by vector

The elementary products XM(IELEM,I) simply have to be replaced by XM(IELEM,I+NLOC*(NLOC-1)/2) if I $\leq$ NLOC*(NLOC-1)/2 and by XM(IELEM,I-NLOC*(NLOC-1)/2) if I $>$ NLOC*(NLOC-1)/2. This gives the following for matrices constructed on the quadrilaterals Q1:

```
W1(IELEM) = + XM(IELEM, 7) * V(I2)
            + XM(IELEM, 8) * V(I3)
            + XM(IELEM, 9) * V(I4)

W2(IELEM) = + XM(IELEM, 1) * V(I1)
            + XM(IELEM,10) * V(I3)
            + XM(IELEM,11) * V(I4)

W3(IELEM) = + XM(IELEM, 2) * V(I1)
            + XM(IELEM, 4) * V(I2)
            + XM(IELEM,12) * V(I4)

W4(IELEM) = + XM(IELEM, 3) * V(I1)
            + XM(IELEM, 5) * V(I2)
            + XM(IELEM, 6) * V(I3)
```

It can be seen from the last two examples above that problems of symmetry and transposition are simply questions of how information is written for non-assembled storage.

5.3.5 Dirichlet-type boundary conditions

The following discussion concentrates on the case in which Dirichlet-type points are not eliminated from the equations. This is the only case that poses any problem, as it calls for local correction of the matrix. Instead of eliminating points that are not degrees of freedom, they are retained and assigned an equation of the type x=prescribed value. In the other equations, 0 is taken as coefficient in places where there is a Dirichlet node, while the right hand sides of the equations are of course also changed. In this way the symmetry of the matrix is not modified.

In other words, for a Dirichlet-type point, 1 is placed on the matrix diagonal and off-diagonal terms are cancelled. Starting from a point, however, there is no data structure for quickly finding elements to which a single point belongs. It is thus apparently impossible to cancel the related off-diagonal terms if these have been stored by element. In spite of this, they may be cancelled with the loop described below, which again uses the principle of the product matrix x vector.
In the following, the vector V has a value of 1 for a normal point and 0 for a Dirichlet point. Thus any element of the matrix that would "touch" a Dirichlet point in a matrix x vector product is cancelled and the other elements remain unchanged, which is the desired effect. For a matrix constructed on quadrilaterals Q1, this gives:

```
DO IELEM=1,NELEM
  I1 = IKLE(IELEM,1)
  I2 = IKLE(IELEM,2)
  I3 = IKLE(IELEM,3)
  I4 = IKLE(IELEM,4)
!
  XM(IELEM, 1) = XM(IELEM, 1) * V(I2) * V(I1)
  XM(IELEM, 2) = XM(IELEM, 2) * V(I3) * V(I1)
  XM(IELEM, 3) = XM(IELEM, 3) * V(I4) * V(I1)
  XM(IELEM, 7) = XM(IELEM, 7) * V(I1) * V(I2)
  XM(IELEM, 4) = XM(IELEM, 4) * V(I3) * V(I2)
  XM(IELEM, 5) = XM(IELEM, 5) * V(I4) * V(I2)
  XM(IELEM, 8) = XM(IELEM, 8) * V(I1) * V(I3)
  XM(IELEM,10) = XM(IELEM,10) * V(I2) * V(I3)
  XM(IELEM, 6) = XM(IELEM, 6) * V(I4) * V(I3)
  XM(IELEM, 9) = XM(IELEM, 9) * V(I1) * V(I4)
  XM(IELEM,11) = XM(IELEM,11) * V(I2) * V(I4)
  XM(IELEM,12) = XM(IELEM,12) * V(I3) * V(I4)
ENDDO
```

In a non-assembled matrix, the row and column for each Dirichlet-type point are thus cancelled, with the exception of the diagonal terms.
As there is a special array for the matrix diagonal, it is then easy to replace an element on this diagonal by 1 whenever the point in question is of Dirichlet type. Similarly, the set values must then be placed in the second members of the linear system.

5.3.6 Products between diagonal matrix and matrix

These products appear in particular during diagonal or block-diagonal preconditioning of a linear system, in which the system matrix M is replaced by DMD, in which D is a diagonal matrix.
It is therefore necessary to obtain the products DM and MD.
In the following FORTRAN examples, D is declared to be a real array of dimension NPOIN and D(I) represents the I^{th} element of the diagonal matrix. As it is obvious how the diagonal of the results matrix is calculated, only the algorithms for the off-diagonal terms will be discussed (case of quadrilaterals Q1):
Product DM:

```
!
DO 1 IELEM = 1 , NELEM
!
  I1 = IKLE(IELEM,1)
  I2 = IKLE(IELEM,2)
  I3 = IKLE(IELEM,3)
  I4 = IKLE(IELEM,4)
```

```
!
  XM(IELEM, 1) = XM(IELEM, 1) * D(I1)
  XM(IELEM, 2) = XM(IELEM, 2) * D(I1)
  XM(IELEM, 3) = XM(IELEM, 3) * D(I1)
!
  XM(IELEM, 4) = XM(IELEM, 4) * D(I2)
  XM(IELEM, 5) = XM(IELEM, 5) * D(I2)
  XM(IELEM, 6) = XM(IELEM, 6) * D(I3)
!
  XM(IELEM, 7) = XM(IELEM, 7) * D(I2)
  XM(IELEM, 8) = XM(IELEM, 8) * D(I3)
  XM(IELEM, 9) = XM(IELEM, 9) * D(I4)
!
  XM(IELEM,10) = XM(IELEM,10) * D(I3)
  XM(IELEM,11) = XM(IELEM,11) * D(I4)
  XM(IELEM,12) = XM(IELEM,12) * D(I4)
!
ENDDO
!
```

The formula for the assembled matrices would be DM(m,n) = D(m) x M(m,n). With XM(IELEM,1) representing for example part of the term M(I1,I2), it is therefore logically multiplied by D(I1). For the product MD, it will be multiplied by D(I2):
<u>Product MD:</u>

```
DO IELEM = 1 , NELEM
!
  I1 = IKLE(IELEM,1)
  I2 = IKLE(IELEM,2)
  I3 = IKLE(IELEM,3)
  I4 = IKLE(IELEM,4)
!
  XM(IELEM, 1) = XM(IELEM, 1) * D(I2)
  XM(IELEM, 2) = XM(IELEM, 2) * D(I3)
  XM(IELEM, 3) = XM(IELEM, 3) * D(I4)
!
  XM(IELEM, 4) = XM(IELEM, 4) * D(I3)
  XM(IELEM, 5) = XM(IELEM, 5) * D(I4)
  XM(IELEM, 6) = XM(IELEM, 6) * D(I4)
!
  XM(IELEM, 7) = XM(IELEM, 7) * D(I1)
  XM(IELEM, 8) = XM(IELEM, 8) * D(I1)
  XM(IELEM, 9) = XM(IELEM, 9) * D(I1)
!
  XM(IELEM,10) = XM(IELEM,10) * D(I2)
  XM(IELEM,11) = XM(IELEM,11) * D(I2)
  XM(IELEM,12) = XM(IELEM,12) * D(I3)
!
ENDDO
```

The result is itself in the form of a non-assembled matrix and the previous two loops are vectorised.

5.3.7 Matrix-vector product with edge-based storage

As matrices in edge-based storage are fully assembled, the matrix-vector product is rather easy to implement. If one wants to multiply a matrix A by a vector Y, to get X, first the diagonal terms have to be taken into account, X is initialised with DA Y. Then the off-diagonal terms are dealt with with the following assembly loop:

```
DO ISEG=1,NSEG
  X(GLOSEG(ISEG,1))=
  X(GLOSEG(ISEG,1))+XA1(ISEG)*Y(GLOSEG(ISEG,2))
!
  X(GLOSEG(ISEG,2))=
  X(GLOSEG(ISEG,2))+XA2(ISEG)*Y(GLOSEG(ISEG,1))
ENDDO
```

For rectangular matrices, all the values of X are not initialised by the diagonal terms, so some terms in X have to be previously set to 0.

5.4 Solvers and preconditioning operations

BIEF offers several iterative methods for solving a linear system M.X=B. This can be done with preconditioning. A single solving subroutine SOLVE (see section A.IV) processes both cases in which M is a matrix and those in which it is a block consisting of 4 or 9 matrices. In the subroutine SOLVE, preconditioning and method are specified by the arguments PRECON and METHOD.
The integer PRECON may have the following values at present:

0 or 1 no preconditioning

2 preconditioning with the matrix diagonal

3 block-diagonal preconditioning

5 diagonal preconditioning with absolute value of matrix diagonal

7 Crout preconditioning

11 : Gauss-Seidel EBE preconditioning

13 : Preconditioning matrix given by the user

17 : 3-diagonal solution on points on a vertical in 3D (specific to TELEMAC-3D)

or a combination of these values. As the basic preconditioning operations are designated by a prime number, it can be split into PRECON prime factors in order to determine the various preconditioning operations required by the user. For example, PRECON=14 corresponds to combined diagonal preconditioning and Crout preconditioning.
METHOD in an array of two integers.
The integer METHOD(1) may have the following values at present:

1 for the conjugate gradient method

2 for the conjugate residualconjugate residual method

3 for the normal equationnormal equation conjugate gradientconjugate gradient method

4 for the minimum errorminimum error method

5 for the squared conjugate gradient method

6 for the stabilised squared conjugate gradient method

7 for the GMRES method

8 for a direct solution

The integer METHOD(2) designates an option or alternative of the selected solver. At present, this is only used for the GMRES method and designates the dimension of the Krylov sub-space. The various solvers and preconditioning operations will now be described in succession.

5.4.1 The various solvers

A direct solver has been added to library BIEF from version 5.8 on (solver number 8). As it may be changed in a near future (replaced by the software called MUMPS) it will not be described here. Only iterative solvers are referred to hereafter.
These are used to solve a linear system of the form A.X = B. It will be recalled that the different methods are chosen by assigning a certain value to the integer METHOD. All the methods are iterative. Starting with an estimate of the solution X0, they construct a series of vectors Xm that converge towards the exact solution of the system (provided of course that A has the required properties).
Preconditioning options 7, 11, 13 and 17 are the only directly involved in the algorithms of the various solution methods. The other types of preconditioning act on the matrix upline of the calculation. A diagonal preconditioning like 2 or 3 may be combined with another preconditioning like 7, 11 and 13. In this case the choice is the product of both, e.g. 14 for a combination of diagonal and Crout preconditioning.
Note: preconditioning 7, 11 and 13 may behave differently in parallel, and are thus not recommended with domain decomposition
The algorithms for the various methods available in BIEF are listed below. (X,Y) designates the scalar product of the vectors X and Y and C is either the identity (no preconditioning) or the Crout preconditioning matrix.

Conjugate gradient method (METHOD=1)

Convergence is ensured if A is a positive symmetrical matrix.
<u>Initialisation operations:</u>
$r^0 = AX^0 - B$
solution of $Cg^0 = r^0$
$d^0 = g^0$
$\rho^0 = \frac{(r^0,g^0)}{(Ad^0,d^0)}$
$X^1 = X^0 - \rho^0 d^0$
<u>Iterations:</u>
$r^m = r^{m-1} - \rho^{m-1} Ad^{m-1}$
solution of $Cg^m = r^m$
$d^m = g^m + \frac{(r^m,g^m)}{(r^{m-1},g^{m-1})} d^{m-1}$
$\rho^m = \frac{(r^m,d^m)}{(d^m,Ad^m)}$
$X^{m+1} = X^m - \rho^m d^m$

Conjugate residual method (METHOD=2)

Convergence is ensured if A is a positive symmetrical matrix.
<u>Initialisation operations:</u>
$r^0 = AX^0 - B$
solution of $Cg^0 = r^0$
$d^0 = g^0$
solution of $Cd'0 = Ad^0$

$\rho^0 = \frac{(g^0, Ad^0)}{(d'^0, Ad^0)}$
$X^1 = X^0 - \rho^0 d^0$
Iterations:
$r^m = r^{m-1} - \rho^{m-1} A d^{m-1}$
$g^m = g^{m-1} - \rho^{m-1} d'^{m-1}$
$d^m = g^m - \frac{(Ag^m, d'^{m-1})}{(Ad^{m-1}, d'^{m-1})} d^{m-1}$
$Ad^m = Ag^m - \frac{(Ag^m, d'^{m-1})}{(Ad^{m-1}, d'^{m-1})} Ad^{m-1}$
solution of $Cd'^m = Ad^m$
$\rho^m = \frac{(Ad^m, g^m)}{(Ad^m, d'^m)}$
$X^{m+1} = X^m - \rho^m d^m$

Normal equation conjugate gradient method (METHOD=3)

Convergence is ensured if A is a regular matrix.
Initialisation operations:
$r^0 = AX^0 - B$
solution of $Cg^0 = r^0$
solution of ${}^tCg'^0 = g^0$
$d^0 = {}^t Ag'^0$
solution of $Cd'^0 = Ad^0$
$\rho^0 = \frac{(d^0, d^0)}{(d'^0, d'^0)}$
$X^1 = X^0 - \rho^0 d^0$
Iterations:
$r^m = r^{m-1} - \rho^{m-1} A d^{m-1}$
$g^m = g^{m-1} - \rho^{m-1} d'^{m-1}$
solution of ${}^tCg'^m = g^m$
$d^m = {}^t Ag'^m + \frac{({}^tAg'^m, {}^tAg''^m)}{({}^tAg'^{m-1}, {}^tAg'^{m-1})} d^{m-1}$
solution of $Cd'^m = Ad^m$
$\rho^m = \frac{({}^tAg'^m, {}^tAg'^m)}{(d'^m, d'^m)}$
$X^{m+1} = X^m - \rho^m d^m$

Minimum error method (METHOD=4)

Convergence is ensured if A is a regular matrix.
Initialisation operations:
$r^0 = AX^0 - B$
solution of $Cg^0 = r^0$
solution of ${}^tCg'^0 = g^0$
$d^0 = {}^t Ag'^0$
$\rho^0 = \frac{(g^0, g^0)}{(d^0, d^0)}$
$X^1 = X^0 - \rho^0 d^0$
Iterations:
$r^m = r^{m-1} - \rho^{m-1} A d^{m-1}$
solution of $Cg^m = r^m$
solution of ${}^tCg'^m = g^m$
$d^m = {}^t Ag'^m + \frac{(g^m, g'^m)}{(g^{m-1}, g^{m-1})} d^{m-1}$
$\rho^m = \frac{(g^m, g^m)}{(d^m, d^m)}$
$X^{m+1} = X^m - \rho^m d^m$

Conjugate gradient squared method (METHOD=5)

The algorithm is presented without preconditioning, as it is implemented in BIEF.
Convergence is ensured if A is a regular matrix.
Initialisation operations:
$g^0 = AX^0 - B$
$k^0 = p^0 = g^0$
Iterations:
$\rho^m = \frac{(k^m, g^0)}{(Ap^m, g^0)}$
$h^m = k^m - \rho^m A p^m$
$X^{m+1} = X^m - \rho^m (h^m + k^m)$
$g^{m+1} = g^m - \rho^m A(h^m + k^m)$
$\beta^m = \frac{(g^{m+1}, g^0)}{(g^m, g^0)}$
$\rho^{m+1} = g^{m+1} + 2\beta^m h^m + (\beta^m)^2 p^m$
$k^{m+1} = g^{m+1} + \beta^m . h^m$
The stop test is the same for all the methods. Iterations continue until EPSI precision specified by the user is reached after the test:
$\frac{\|A.X^{m+1} - B\|}{\|B\|} \leq EPSI$ if $\|B\| \geq 1$.(relative precision)
or
$\|A.X^{m+1} - B\| \leq EPSI$ if $\|B\| < 1$.(relative precision)

Conjugate gradient squared stabilised (METHOD=6)

This technique is a variant of the conjugate gradient squared method. It has been programmed in BIEF by the University of Hannover (R. Ratke and A. Malcherek).

Generalised minimum residual =GMRES (METHOD=7)

The GMRES method has been published in 1983 and was a great improvement for non-symmetrical complex linear systems. We shall only give here the basic idea, to explain what is the dimension of KRYLOV space. As a matter of fact, this dimension is the component KRYLOV of SLVCFG structures in BIEF.
At every iteration n of the algorithm, we try to minimise $|AX - B|$. This would give the exact solution if X were sought for in the whole space, but here we restrict the investigation to the so-called Krylov subspace generated by $r = AX^n - B, Ar, A^2r, ..., A^{k-1}r$. k is the dimension of this space.
How to minimise $AX - B$ in such a space will not be detailed here. We shall just consider 2 consequences of the method:

1. At every iteration, we have k matrix-vector to build, compared to 1 with the conjugate gradient method, and 2 with the Normal equation technique.

2. If A is a diagonal, the Krylov space will degenerate and the method will fail.

5.4.2 Diagonal preconditioning

The problem here involves solving a linear system of the form MX=B.
"Point diagonal" preconditioning means preconditioning in the etymological sense of the term, as it really applies before the system is solved. The diagonal matrix D is formed, such that:
$D(i,i) = \frac{1}{\sqrt{M(i,i)}}$ (PRECON = 2 or 3) $D(i,i) = \frac{1}{\sqrt{|M(i,i)|}}$ (PRECON = 5)
M(i,i) must therefore be non-zero or even positive, as appropriate.
The following equation is then solved:
$DMDD^{-1}X = DB$

This produces:
a new matrix: $M' = DMD$
a new unknown vector: $X' = D^{-1}X$
a new right hand side: $B' = DB$
By construction in cases where M(i,i) is always positive, the diagonal of M' consists of only 1 (this fact may be exploited by SOLVE for optimisation purposes). The effect of preconditioning is thus to assign a comparable importance to all the equations.
Once the system M'X' = B' has been solved, it is easy to find X, which is equal to DX'.
This illustrates the advantage, with the EBE storage system, of having assembled the matrix diagonal, which makes it easy to calculate D.
N.B. Other choices could be made for the diagonal D. This possibility is exploited internally in BIEF, for example for block-diagonal preconditioning.

5.4.3 Block-diagonal preconditioning

This type of preconditioning is only meaningful when the matrix M is a block of squared matrices. Detailed explanations are given below for an example with a block of 4 atrices:

Case of a block of 4 matrices

The problem is to solve a system MX=B, in which:

$$M = \begin{vmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{vmatrix}, X = \begin{vmatrix} X_1 \\ X_2 \end{vmatrix} and B \begin{vmatrix} B_1 \\ B_2 \end{vmatrix}$$

D_{11}, D_{12}, D_{21}, and D_{22} will be used to designate the respective diagonals of M_{11}, M_{12}, M_{21}, and M_{22}.
The basic idea is to obtain an approximate solution for M using the matrix: $\tilde{M} = \begin{vmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{vmatrix}$
and an LDU decomposition of in the form $L\sqrt{D}\sqrt{D}U$. The initial system MX=B is thus changed into: $\left(L\sqrt{D}\right)^{-1} M \left(\sqrt{D}U\right)^{-1} \sqrt{D}UX = \left(L\sqrt{D}\right)^{-1} B$
By expansion, this system can also be written as:
$\frac{1}{\sqrt{D}} L^{-1} M U^{-1} \frac{1}{\sqrt{D}} \sqrt{D}UX = \frac{1}{\sqrt{D}} L^{-1}$
In this form, the system appears as a diagonal preconditioning of the system AX' = B', with a given preconditioning diagonal D and assuming:
$A = L^{-1}MU^{-1}$
$X' = UX$
$B' = L^{-1}B$
Having solved the system, the unknown X can be obtained by the formula $X = U^{-1}X'$.
The following operations must therefore be carried out in sequence:

1. Calculation of L, D and U by LDU decomposition of $\tilde{M} = \begin{vmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{vmatrix}$
2. Calculation of A, X' and B'
3. Solution of the system A X' = B' with simple diagonal preconditioning, in which the diagonal D is specified (see previous section).
4. Calculation of X as a function of X'.

Operations 1, 2 and 4 will now be described in detail:

1. LDU decomposition of $\tilde{M} = \begin{vmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{vmatrix}$

   $\widetilde{M}$ is broken down in the form $\begin{vmatrix} I & 0 \\ L_{21} & I \end{vmatrix} \begin{vmatrix} D'_{11} & 0 \\ 0 & D'_{22} \end{vmatrix} \begin{vmatrix} I & U_{12} \\ 0 & I \end{vmatrix}$

   By identification:

   $D'_{11} = D_{11}$

   $L_{21} = \frac{D_{21}}{D_{11}}$

   $U_{12} = \frac{D_{12}}{D_{11}}$

   $D'_{22} = D_{22} - L_{21} D_{11} U_{12}$

   In practice, programming will be done by combining the following diagonals in the memory:

   D'_{11} and D_{11} D'_{22} and D_{22} L_{21} and D_{21} U_{12} and D_{12}

   This is done with the successive operations:

   $D_{21} = \frac{D_{21}}{D_{11}}$

   $D_{22} = D_{22} - D_{21} D_{12}$

   $D_{12} = \frac{D_{12}}{D_{11}}$

   $\widetilde{M}$ is thus $\begin{vmatrix} I & 0 \\ D_{21} & I \end{vmatrix} \begin{vmatrix} D_{11} & 0 \\ 0 & D_{22} \end{vmatrix} \begin{vmatrix} I & D_{12} \\ 0 & I \end{vmatrix}$

   The diagonals D_{11} and D_{22} are inverted and the square root extracted. They are then kept for subsequent diagonal preconditioning (operation 3). They are no longer used for operations 2 and 4.

2. Calculation of A, X' and B'

   The following formulae are used:

   $$\begin{vmatrix} I & 0 \\ D_{21} & I \end{vmatrix}^{-1} = \begin{vmatrix} I & 0 \\ -D_{21} & I \end{vmatrix}$$

   and:

   $$\begin{vmatrix} I & D_{12} \\ 0 & I \end{vmatrix}^{-1} = \begin{vmatrix} I & -D_{12} \\ 0 & I \end{vmatrix}$$

   The product $\begin{vmatrix} I & 0 \\ -D_{21} & I \end{vmatrix} \begin{vmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{vmatrix}$ is equal to $\begin{vmatrix} M_{11} & M_{12} \\ M_{21} - D_{21} M_{11} & M_{22} - D_{21} M_{12} \end{vmatrix}$

   As for LDU decomposition, A will be calculated "in situ" by using M.

   The following operations are therefore performed first of all:

   $M_{21} = M_{21} - D_{21} M_{11}$ and $M_{22} = M_{22} - D_{21} M_{12}$

   Right-hand multiplication by U^{-1} is then done by the following operations:

   $M_{12} = M_{12} - M_{11} U_{12}$ and $M_{22} = M_{22} - M_{21} U_{12}$

   On completion of these operations, the matrix A takes the place of M.

   X' is also calculated in situ by the operation: $X_1 = X_1 + D_{12} X_2$ (X_2 remains unchanged).

   B' is calculated by the operation: $B_2 = B_2 - D_{21} B_1$ (B_1 remains unchanged).

4. Calculation of X

   This is done by the single operation: $X_1 = X_1 - D_{12} X_2$ (X_2 remains unchanged).

Case of a block of 9 matrices

The problem is to solve the system MX=B, in which:

$$M = \begin{vmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{vmatrix}, X = \begin{vmatrix} X_1 \\ X_2 \\ X_3 \end{vmatrix} and B = \begin{vmatrix} B_1 \\ B_2 \\ B_3 \end{vmatrix}$$

D_{ij} will be used to designate the respective diagonals M_{ij}.

The preconditioning principle is exactly the same as for a block of 4 matrices.

The following operations must therefore be carried out in sequence:

1. Calculation of L, D and U by LDU decomposition of: $\tilde{M} = \begin{vmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{vmatrix}$
2. Calculation of A, X' and B'
3. Solution of the system A X' = B' with a single preconditioning diagonal, in which the diagonal D is specified (see previous section).
4. Calculation of X as a function of X'.

Operations 1, 2 and 4 will now be described in detail:

1. LDU decomposition of $\tilde{M} = \begin{vmatrix} D_{11} & D_{12} & D_{13} \\ D_{21} & D_{22} & D_{23} \\ D_{31} & D_{32} & D_{33} \end{vmatrix}$ $\tilde{M}$ is broken down in the form

   $$\begin{vmatrix} I & 0 & 0 \\ D'_{21} & I & 0 \\ D'_{31} & D'_{32} & I \end{vmatrix} \begin{vmatrix} D'_{11} & 0 & 0 \\ 0 & D'_{22} & 0 \\ 0 & 0 & D'_{33} \end{vmatrix} \begin{vmatrix} I & D'_{12} & D'_{13} \\ 0 & I & D'_{23} \\ 0 & 0 & I \end{vmatrix}$$

   In situ decomposition, in which the values D' and D are combined, involves the following operations:

   D_{11} is unchanged.

   D_{21} is replaced by $\frac{D_{21}}{D_{11}}$

   D_{31} is replaced by $\frac{D_{31}}{D_{11}}$

   D_{22} is replaced by $D_{22} - D_{21}D_{11}D_{12}$

   D_{32} is replaced by $\frac{D_{32}-D_{31}D_{12}}{D_{22}}$

   D_{23} is replaced by $D_{23} - D_{13}D_{21}$ (Division by D_{22} deliberately omitted)

   D_{33} is replaced by $D_{33} - D_{31}D_{13} - D_{32}D_{23}$ (D_{23} is in fact D_{22} D_{23} here)

   D_{12} is replaced by $\frac{D_{12}}{D_{11}}$

   D_{13} is replaced by $\frac{D_{13}}{D_{11}}$

   D_{23} is replaced by $\frac{D_{23}}{D_{22}}$ (to rectify previous omission)

   The divisions are in fact replaced by multiplications by prior inversion of the diagonals D_{11}, D_{22} and D_{33}, which will only be used in this form afterwards. The square root is then extracted after inversion and they are kept for diagonal preconditioning.

2. Calculation of A, X' and B'

   The following formulae are used:

$$\begin{vmatrix} I & 0 & 0 \\ D_{21} & I & 0 \\ D_{31} & D_{32} & I \end{vmatrix}^{-1} = \begin{vmatrix} I & 0 & 0 \\ 0 & I & 0 \\ -D_{31} & -D_{32} & I \end{vmatrix} \begin{vmatrix} I & 0 & 0 \\ -D_{21} & I & 0 \\ 0 & 0 & I \end{vmatrix}$$

and

$$\begin{vmatrix} I & D_{12} & D_{13} \\ 0 & I & D_{23} \\ 0 & 0 & I \end{vmatrix}^{-1} = \begin{vmatrix} I & -D_{12} & 0 \\ 0 & I & 0 \\ 0 & 0 & I \end{vmatrix} \begin{vmatrix} I & 0 & -D_{13} \\ 0 & I & -D_{23} \\ 0 & 0 & I \end{vmatrix}$$

These two breakdown operations are used to calculate A, bearing in mind that M is multiplied on the left by the lower part and on the right by the upper part. *In situ* modifications are made to the matrix:

Left-hand multiplication is done by means of the following operations:

M_{21} is replaced by $M_{21} - D_{21}M_{11}$

M_{22} is replaced by $M_{22} - D_{21}M_{12}$

M_{23} is replaced by $M_{23} - D_{21}M_{13}$

M_{31} is replaced by $M_{31} - D_{31}M_{11} - D_{32}M_{21}$

M_{32} is replaced by $M_{32} - D_{31}M_{12} - D_{32}M_{22}$

M_{33} is replaced by $M_{33} - D_{31}M_{13} - D_{32}M_{23}$

Right-hand multiplication is done by means of the following operations:

M_{12} is replaced by $M_{12} - M_{11}D_{12}$

M_{22} is replaced by $M_{22} - M_{21}D_{12}$

M_{32} is replaced by $M_{32} - M_{31}D_{12}$

M_{13} is replaced by $M_{13} - M_{11}D_{13} - M_{12}D_{23}$

M_{23} is replaced by $M_{23} - M_{21}D_{13} - M_{22}D_{23}$

M_{33} is replaced by $M_{33} - M_{31}D_{13} - M_{32}D_{23}$

On completion of these operations, the matrix A thus takes the place of M. X' is also calculated *in situ* by the operations:

$X_1 = X_1 + D_{12}X_2 + D_{13}X_3$

$X_2 = X_2 + D_{23}X_3$

X_3 remains unchanged.

B' is calculated by the operations:

$B1$ remains unchanged.

$B_2 = B_2 - D_{21}B_1$

$B_3 = B_3 - D_{31}B_1 - D_{32}B_2$

3. Calculation of X

   This is done by the operations:

   X_3 remains unchanged.

   $X_2 = X_2 - D_{23}X_3$

   $X_1 = X_1 - D_{12}X_2 - D_{13}X_3$

5.4.4 LU preconditioning

Two matrices L and U (lower and upper) are chosen so that the product LU is close to A. The choice of L and U of course determines the efficiency of preconditioning and examples will be given in the following sections. For the moment, L and U will be assumed to have known values.
In place of the system M X = B, the following equivalent system is solved:
$L^{-1}MU^{-1}UX = L^{-1}B$
This produces:
a new matrix: $M' = L^{-1}MU^{-1}$
a new unknown vector: $X' = UX$
a new second member: $B' = L^{-1}B$
After solving this system, X is obtained by the formula $X = U^{-1}X'$
When M is symmetrical, it is preferable to choose an LU breakdown in which L and U are each transposed from the other. In the case of $LU = L^tL$ iterative methods such as that of the conjugate gradient (see Solvers may be adapted to produce only one inversion by $(L^tL)^{-1}$. See J.-M. [2] on this subject.

5.4.5 CROUT preconditioning

Principle

In this case, the aim is to obtain a decomposition close to M in the form $N = LDU$, in which L and U are respectively lower and upper, with the identity as diagonal.
Assuming that the diagonal of M is the identity (if this is not the case, it is simply a question of applying a diagonal preconditioning before Crout preconditioning, provided that the diagonal of M allows this). M is then written as a function of the elementary matrices E_e:

$$M = I + \sum_{e=1}^{NELEM} P_e E_e P_e^t$$

To obtain an approximation of M, the aim is to apply the identity: $1 + \sum_i \varepsilon_i \approx \prod_i (1 + \varepsilon_i)$ with small values of ε_i. This gives: $M = \prod_{e=1}^{NELEM} (I + P_e E_e P_e^t)$
E_e is a zero-diagonal matrix. Introducing:
$\overline{E}_e$ with the diagonal as identity, equal to the matrix Ee for the off-diagonal terms.
$\overline{E}_e = E_e + I_e$ (Ie elementary-level identity).
$\overline{I}_e$ equal to I with zeros on the diagonal at positions corresponding to the nodes of element e.
$\overline{I}_e = I - P_e L_e P_e^t$.
Crout's decomposition is then applied to $\overline{E}_e$, hence:$\overline{E}_e = L_e D_e E_e$.
in which L_e is a lower triangular matrix with the identity as diagonal, De a diagonal matrix and Ue an upper triangular matrix with the identity as diagonal. The approximate expression for M becomes:

$$M = \prod_{e=1}^{NELEM} (\tilde{I}_e + P_e(L_e D_e U_e) P_e^t)$$

Lastly, a similar expression, written symmetrically, is used for N:

$$N = \prod_{e=1}^{NELEM} (\tilde{I}_e + P_e(L_e)P_e^t) \prod_{e=1}^{NELEM} (\tilde{I}_e + P_e(D_e)P_e^t) \prod_{e=NELEM}^{1} (\tilde{I}_e + P_e(U_e)P_e^t)$$

The product $\prod_{e=1}^{NELEM} (\tilde{I}_e + P_e(D_e)P_e^t)$ which is a diagonal matrix that will by designated D, is easy to calculate.
A linear system of the form $N.X = B$ is thus solved by a succession of forward and backward sweeps, firstly on the upper triangular matrices Ue and then, having inverted the diagonal matrix D, on the lower triangular matrices L_e.

Example with triangles P1

The matrix M is given by its diagonal DM(NPOIN), which is the identity, and its off-diagonal terms XM(NELEM,6) (M is not assumed to be symmetrical).

LDU breakdown

The elementary matrices are broken down into LDU products by applying Crout's algorithm. The result is stored for the matrices De in DN(NPOIN) after assembly by multiplication and for Le and Ue in XN(NELEM,6).

Crout's algorithm applied to a matrix (aij) (1≤i,j≤n) is then written as follows:

- If j=1,n then:
  - If i=1,j then:
    $\beta_{ij} = a_{ij} - \sum_{k=1}^{i-1} \alpha_{ik}\beta_{kj}$ (if i=1, the summation is 0)
- and
  - If i=j+1,n then:
    $\alpha_{ij} = \frac{1}{\beta_{jj}}(a_{ij} - \sum_{k=1}^{j-1} \alpha_{ik}\beta_{kj})$ (if i=1, the summation is 0)

An LU breakdown is thus obtained (L consisting of the α_{ij} and U of the β_{ij} values). LDU breakdown is then obtained by dividing each β_{ij} by β_{ii}:

L lower triangular matrix: $L_{ij} = \alpha_{ij}(j < i), L_{ii} = 1, L_{ij} = 0(i < j)$

D diagonal matrix: $D_{ii} = \beta_{ii}$

U upper triangular matrix: $U_{ij} = \beta_{ij}(j < i), U_{ii} = 1, U_{ij} = \beta_{ij}/\beta_{ii}(i < j)$

In FORTRAN, this gives:

```
!
        DO IELEM=1,NELEM
!
! MATRIX TO BE BROKEN DOWN ( WITH VALUES 1 ON THE DIAGONAL)
!
! LINE 1
           A11 = 1.D0
           A12 = XM(IELEM,1)
           A13 = XM(IELEM,2)
! LINE 2
           A21 = XM(IELEM,4)
           A22 = 1.D0
           A23 = XM(IELEM,3)
! LINE 3
           A31 = XM(IELEM,5)
           A32 = XM(IELEM,6)
           A33 = 1.D0
!
! CROUT L*U DECOMPOSITION
!
! ROW 1 (BETA11=1)
           ALFA21 = A21
           ALFA31 = A31
!
! ROW 2
           BETA12 =  A12
           BETA22 =  A22 - ALFA21*BETA12
           ALFA32 = (A32 - ALFA31*BETA12)/BETA22
```

```
!
! ROW 3
           BETA13 =  A13
           BETA23 =  A23 - ALFA21*BETA13
           BETA33 =  A33 - ALFA31*BETA13 - ALFA32*BETA23
!
! L*D*U BREAK DOWN
! THE EXTRA DIADONAL TERMS AND W2,W3 ARE STORED IN XN  (W1 IS NOTC USED BECAUSE BETA1
!
           XN(IELEM,1)  = BETA12
           XN(IELEM,2)  = BETA13
           XN(IELEM,3)  = BETA23/BETA22
!
           XN(IELEM,4)  = ALFA21
           XN(IELEM,5)  = ALFA31
           XN(IELEM,6)  = ALFA32
!
           W2(IELEM)     = BETA22
           W3(IELEM)     = BETA33
!
        ENDDO
!
```

The matrix L is stored in XN(IELEM,4), XN(IELEM,5) and XN(IELEM,6), matrix U in XN(IELEM,1), XN(IELEM,2) and XN(IELEM,3) and arrays W2 and W3 are assembled by multiplication in DN (previously initialised at 1) as follows:

```
!----------------------------------------------------------------------
! LOOP WITH FORCED VECTORISATION
!----------------------------------------------------------------------
!
!DIR$ IVDEP
      DO 10 IELEM = 1 , NELEM
        DN(IKLE(IELEM,2)) = DN(IKLE(IELEM,2)) * W2(IELEM)
10    CONTINUE
!
!DIR$ IVDEP
      DO 20 IELEM = 1 , NELEM
        DN(IKLE(IELEM,3)) = DN(IKLE(IELEM,3)) * W3(IELEM)
20    CONTINUE
!
```

The loop appearing in the multiplying assembly may be vectorised for the same reasons as in a conventional assembly. The vector DN is then inverted, as N^{-1} is the point of interest.

```
!
!  DN INVERSION
!
      CALL OV( 'X=1/Y   ' , DN , DN , Z , C , NPOIN )
```

Inversion of system N.X = B

```
!-----------------------------------------------------------------------
!
!  INITIALISATION: X = RIGHT HAND SIDE
!
      CALL OV( 'X=Y     ' , X , B , Z , C , NPOIN )
!
```

```
!-----------------------------------------------------------------------
!
! SERIE OF LOWER TRIANGULAR MATRICES INVERSION
!
!DIR$ IVDEP
       DO IELEM = 1 , NELEM
!
      X(IKLE(IELEM,2)) = (X(IKLE(IELEM,2))
     &           - XN(IELEM,4) * X(IKLE(IELEM,1)) )
!
      X(IKLE(IELEM,3)) = ( X(IKLE(IELEM,3))
     &           - XN(IELEM,5) *  X(IKLE(IELEM,1))
     &           - XN(IELEM,6) *  X(IKLE(IELEM,2)) )
!
 30      CONTINUE
!
! MULTIPLICATION BY DN (ALREADY INVERTED)
        CALL OV( 'X=XY    ' , X , DN , Z , C , NPOIN )
!
! SERIE OF UPPER TRIANGULAR MATRICES INVERSION
!
!DIR$ IVDEP
        DO IELEM = NELEM , 1 , -1
!
      X(IKLE(IELEM,2)) = ( X(IKLE(IELEM,2))
     &           - XN(IELEM,3) *  X(IKLE(IELEM,3)) )
!
      X(IKLE(IELEM,1)) = ( X(IKLE(IELEM,1))
     &         - XN(IELEM,1) *  X(IKLE(IELEM,2))
     &         - XN(IELEM,2) *  X(IKLE(IELEM,3)),)
!
        ENDDO
!
!-----------------------------------------------------------------------
!
```

Loops 1 and 2 cannot normally be vectorised, even with the precautions taken to vectorise the vector assembly. Indeed, this would require IKLE(IELEM1,I) $\neq$ IKLE(IELEM2,J) for I,J = 1,2,3 for all different elements IELEM1, IELEM2 taken in a cluster of e.g. 64 elements , and this condition is only achieved for I=J in the grids used here. Nevertheless, forced vectorisation may be considered. The result obtained in this way will certainly not be a solution of N.X = B, but it should not be forgotten that the aim of constructing N was to obtain an approximation of M, i.e. an approximate solution of M.X = B. It is therefore quite acceptable to take the result with forced vectorisation for this purpose. In any case, as will be seen below, there is stop test at the end of any iterative method, ensuring that a good solution has been obtained. Tests show that Crout's preconditioner is particularly effective when it can be applied. For diffusion matrices, the computation cost can be reduced by 50% in spite of the time spent in constructing the preconditioner.

5.4.6 GAUSS-SEIDEL EBE PRECONDITIONING

The principle is similar to that of Crout preconditioning. Assuming that the diagonal of M is the identity, L is chosen equal to the lower part of M and with an identity diagonal, and U equal to the upper part of M, with an identity diagonal. Thus:
$L+U = M+I$

Once this choice has been made, the forward and backward sweep principle is the same as for Crout preconditioning.

6. How to implement reproducibility in openTelemac

In [5] and [6], we analyse and obtain the numerical reproducibility of *gouttedo* and *Nice*, two test cases of the modules TELEMAC-2D and TOMAWAC, by using the compensation techniques. To obtain a full reproducibility, *i.e.* in all openTelemac modules, these techniques have to be integrated in other computations that differ between the sequential execution and the parallel one. To facilitate such a task, this chapter aims to be a useful technical document. We start describing in Section 6.1 the methodology to track the computation of the concerned problem. This process aims to identify the sources which produce the non-reproducibility. Then, we detail the modifications introduced in the code. As already mentioned, openTelemac relies on its finite element library BIEF. This one includes many Fortran 90 subroutines which provide the data structure, the building and the solving phases of the simulation. Almost all our modifications have been restricted to these library subroutines. We describe four types of modification: data structure, algebraic operations, building phase and solving phase. We exhibit and explain the modified parts highlighting them and commenting them in the listings proposed along the chapter.
The users choose between the original computation or a reproducible one, in the test case file (where all the parameters of the simulation are defined) via the keyword "FINITE ELEMENT ASSEMBLY" (or "ASSEMBLAGE EN ELEMENTS FINIS" in French). It corresponds to the Fortran variable `MODASS` that takes the values 1,2 and 3 respectively for the original, the integer and the compensated mode. In this chapter we only consider the implementation of the compensated computation.

6.1 Methodology

We describe how to identify the source of non-reproducibility in a computation sequence. The strategy is to observe the components of the linear system as the computation is progressing. For that, we introduce the subroutine `glob_vec` to observe the reproducibility of a concerned vector after each computation, see Listing 6.1. This process allows us to detect if a computation is reproducible or not.
In a parallel simulation, the vectors are distributed over the sub-domains where each node has a local and a global number. In order to compare the component values when the sub-domain number differs, we need to rebuild the global vector, *i.e.* for the whole domain. For that we use the structure `KNOLG` which maps the local number of a component to the global one. This treatment is realized in lines from 18 to 29.
As detailed in [5] and [6], reproducibility can be observed only after the interface point assem-

bly (and the compensation), because the interface points are different for one decomposition to another.
For that, in our observation we identify if the interface point assembly has been already performed in lines 8 and 10 of Listing 6.1. If it is not the case, we call the assembly processing `parcom` or `parcom_comp`, corresponding to the computation mode. (we note that the test are realized on a copy of the component, line 4). In the compensated mode (`MODASS`=3), the sequential and the parallel cases both benefit from the compensation, lines 44 and 12 respectively .

Listing 6.1: The BIEF_OBJ structure in `glob_vec`

```
!Input: X is the observed vector, if FLAG_ASS is true an
!interface point assembly is performed
!Copy the concerned vector to a temporary one
CALL OS('X=Y     ',X=MESH%T,Y=X)
!In parallel case
IF (NCSIZE .NE. 0) THEN
  IF (MODASS .EQ. 1) THEN
    IF(FLAG_ASS) CALL PARCOM(MESH%T,2,MESH)
  ELSEIF (MODASS .EQ. 3) THEN
    IF(FLAG_ASS)  THEN
      CALL PARCOM_COMP(MESH%T,MESH%T%E,2,MESH)
      MESH%T%R=MESH%T%R+MESH%T%E
    ENDIF
  ENDIF
!Procedure to obtain the global vector
!which is distributed over the sub-domains
!Each sub-domain stores its maximum local point
  NPOIN_GLOBAL=MAXVAL(MESH%KNOLG%I)
!Sub-domains exchange their maximal local points to store the maximal,
!which represents the number of nodes in the whole domain
  NPOIN_GLOBAL=P_IMAX(NPOIN_GLOBAL)
  ALLOCATE(VALUE_GLOBAL(NPOIN_GLOBAL))
  VALUE_GLOBAL(:)=HUGE(1.D0)
  DO I=1,NPOIN
     VALUE_GLOBAL(MESH%KNOLG%I(I))=MESH%T%R(I)
  END DO
  DO I=1,NPOIN_GLOBAL
     VALUE_GLOBAL(I)=P_DMIN(VALUE_GLOBAL(I))
  END DO
!Write the result by the master sub-domains in a file
  IF (IPID .EQ. 0) THEN
    OPEN(UNIT=99,FILE='./'//X%NAME//'VEC_GLOBAL.TXT')
    WRITE(99,*)  X%NAME,", NB POINTS:",NPOIN_GLOBAL
    DO I=1,NPOIN_GLOBAL
      WRITE(99,*) VALUE_GLOBAL(I)
      CALL FLUSH(99)
    END DO
    CLOSE(99)
  END IF
  CALL P_SYNC
!In sequential case, write the results in a file
ELSE
  IF ((MODASS .EQ.3) .AND. FLAG_ASS)THEN
    MESH%T%R=MESH%T%R+MESH%T%E
  ENDIF
```

```
   OPEN(UNIT=99,FILE='./'//X%NAME//'VEC_GLOBAL.TXT')
   WRITE(99,*) X%NAME,", NB POINTS:",NPOIN
   DO I=1,NPOIN
      WRITE(99,*) MESH%T%R(I)
      CALL FLUSH(99)
   END DO
   CLOSE(99)
END IF
```

6.2 Modifications in the data structure

The main data type in the BIEF library is `BIEF_OBJ` which may be a vector, a matrix or a block. The part of the subroutine `bief_def` in Listing 6.2 illustrates some of the vector and matrix structure types.
We write `V%R` the R component of the vector V which corresponds to the data. In the compensated version, these R values will be associated, when necessary, with the accumulation of the corresponding generated rounding errors. These errors will be stored in a component named E, and we write `V%E` to access to it. The same notations exist for a diagonal D of the matrix M: we write `M%D%R` for the data and `M%D%E` for the errors. The component E accumulates the generated rounding errors in each computation with R, this latter will be corrected by a compensation $R+E$.

Listing 6.2: The BIEF_OBJ structure in `bief_def`

```
! Structures in the object BIEF_OBJ:
TYPE BIEF_OBJ
  INTEGER TYPE            ! 2: vector,  3: matrix,  4: block
  CHARACTER(LEN=6) NAME   ! Name of the object
! For vectors
  INTEGER NAT             ! 1:DOUBLE PRECISION  2:INTEGER
  INTEGER ELM             ! Type of element
  INTEGER DIM1            ! First dimension
  INTEGER DIM2            ! Second dimension
! Double precision vector
! Data are stored here
  DOUBLE PRECISION,POINTER,DIMENSION(:)::R
 ! Errors are stored here
     DOUBLE PRECISION, POINTER,DIMENSION(:)::E
! For matrices
! 1: EBE storage  3: EDGE-BASED storage
  INTEGER STO
! Pointer to a BIEF_OBJ for the diagonal
  TYPE(BIEF_OBJ),POINTER :: D
! Pointer to a BIEF_OBJ for extra-diagonal terms
  TYPE(BIEF_OBJ),POINTER :: X
END TYPE BIEF_OBJ
```

Note 1. The new component `V%E` is allocated in the subroutine `bief_allvec`.

Note 2. When the routine parameters only include `BIEF_OBJ` type, our modifications are automatically available in the body of the subroutine: all the structure components are accessible as `V%R` or `V%E`. Nevertheless, some subroutines work directly with double precision vectors that used to pass an object's component, as `V%R`. In this case, we have to modify the subroutine parameter by manually adding a supplementary one for `V%E`.

6.3 Modifications in the algebraic operations

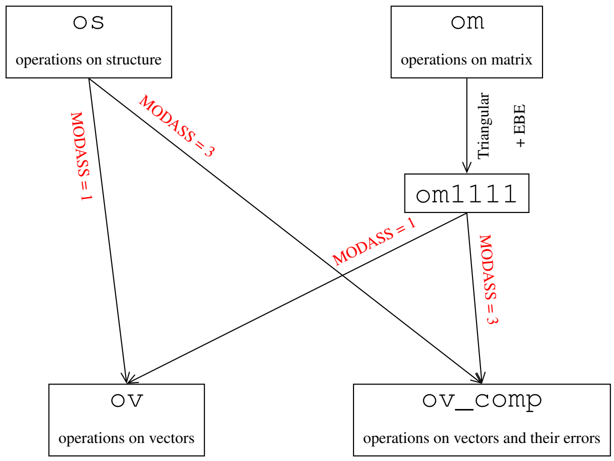
In [6], we explain how the rounding errors `V%E` must be updated for each algebraic operation on `V%R`. Every operation on a block or a vector is called by the subroutine `os`, which only verifies the structure before calling the subroutine `ov`. This latter computes the required operation *op* on the passed vectors `X%R`, `Y%R`, `Z%R`, for instance it computes `X%R = Y%R + Z%R`.
In the compensated mode, the new subroutine `ov_comp` is called, and the passed vectors are associated with their own error vectors `X%E`, `Y%E`, `Z%E`, to also update them. Listing 6.3 illustrates the modified vector add and the Hadamard product, for instance.

Listing 6.3: The algebraic operations in `ov_comp`

```
!X,Y and Z represent the values
!!X_ERR,Y_ERR and Z_ERR represent the errors
!For initialization
CASE('0      ')
DO I=1,NPOIN
   X(I) = 0.D0
    X_ERR(I)=0.D0
ENDDO
!Copy Y to X
CASE('Y      ')
DO I=1,NPOIN
  X(I) = Y(I)
   X_ERR(I) = Y_ERR(I)
ENDDO
!Add two vectors
!In the original code is X(I) = Y(I) + Z(I)
DO I=1,NPOIN
   CALL TWOSUM(Y(I),Z(I),X(I),ERROR)
   X_ERR(I)=(Y_ERR(I)+Z_ERR(I))+ERROR
ENDDO
!Value by value product
!In the original code is X(I) = Y(I) * Z(I)
DO I=1,NPOIN
  CALL TWOPROD(Y(I),Z(I),X(I),ERROR)
  X_ERR(I)=(Y(I) * Z_ERR(I))+(Y_ERR(I) * Z(I))
&          +(Y_ERR(I) * Z_ERR(I))
  X_ERR(I)=X_ERR(I)+ ERROR
ENDDO
```

All these operations are also applied to the diagonal and the extra-diagonal terms of the EBE matrix structure, respectively stored as vectors in `M%D` and `M%X`. The difference is in the sequence of the calls, which begin by the subroutine `om` for matrix instead of `os` for other structures. In `om`, the storage and the type of the element are verified to call the subroutine `om1111` for triangular elements and EBE storage. In this subroutine, several tests are verified to then pass the corresponding component vector of the matrix to the subroutines `ov` or `ov_comp`. In the compensated version, the only modification in `om` and `om1111` is at the subroutine parameter level to pass the error vectors.

Figure 6.1: A general scheme of the algebraic operation calls



6.4 Modifications in the building phase

As detailed in [6], the steps of the building phase which condition the reproducibility are the finite element assembly and its complement in parallel, the interface node assembly. In the compensated mode, the generated rounding errors of an elementary addition are calculated by the subroutine `2sum` which is added in BIEF. In practice, the computation of any vector is realized in the subroutine `vectos`. Listing 6.4 is a part of this subroutine and we detail it in three steps.

Listing 6.4: The call of the FE assembly under the two modes of the computation in `vectos`

```
! Note: VEC is a reference to SVEC%R
IF(MODASS.EQ.1) THEN
   CALL ASSVEC(VEC, IKLE, NPT ,NELEM,NELMAX,IELM1,
&    T,INIT,LV,MSK,MASKEL,NDP)
ELSEIF(MODASS.EQ.3 ) THEN
  CALL ASSVEC(VEC, IKLE, NPT ,NELEM,NELMAX,IELM1,
&   T,INIT,LV,MSK,MASKEL,NDP,SVEC%E)
ENDIF
! Implicit modification in PARCOM
IF(ASSPAR) CALL PARCOM(SVEC,2,MESH)
IF(ASSPAR.AND.MODASS.EQ.3) THEN
! The compensation of all the values
  DO I = 1 , MESH%NPOIN
      VEC(I)= VEC(I)+SVEC%E(I)
  ENDDO
ENDIF
```

1. `vectos` calls the subroutine `assvec` that computes the finite element assembly process corresponding to the computation mode, from line 2 to 8. In the original mode, only the vector `VEC` is passed into the `assvec` call, while in the compensated mode, we also pass the vector of errors `SVEC%E`.

Listing 6.5: The FE assembly in `assvec`

```
!X refers to VEC and ERRX refers to SVEC%E
DO IDP = 1 , NDP
  DO IELEM = 1 , NELEM
```

```
    IF (MODASS.EQ.1)
 &   X(IKLE(IELEM,IDP)=X(IKLE(IELEM,IDP)+W(IELEM,IDP)
    ELSEIF (MODASS.EQ.3) THEN
      CALL 2SUM(X(IKLE(IELEM,IDP)),
    &    W(IELEM,IDP),X(IKLE(IELEM,IDP)),ERROR)
      ERRX(IKLE(IELEM,IDP))=ERRX(IKLE(IELEM,IDP))+ERROR
    ENDIF
  ENDDO
ENDDO
```

As showed in Listing 6.5, only the vector VEC is assembled in the original computation (line 5). In the compensated mode, VEC is assembled by the subroutine 2sum (lines 7 and 8) that also computes the rounding error ERROR for each node IKLE(IELEM,IDP). The vector SVEC%E accumulates the generated errors ERROR of each node.

2. The second implicit modification in Listing 6.4 (line 10) is the interface node assembly that is launched by the subroutine parcom. This later calls parcom2, which then calls paraco twice in the original mode. We recall that the first call is to assemble the sub-domain contributions and the second is to recover the solution continuity between the sub-domains by sharing their maximum value (this choice is justified by physical reasons in [1]).
In the compensated mode, parcom2_comp and paraco_comp replace parcom2 and paraco, respectively.
The modification in parcom_comp are the addition of the error component parameter and the suppression of the second call of paraco which is no more need because our corrections recover the solution continuity between the sub-domains.
The main modifications occur in paraco_comp and are presented in Listing 6.6. The Fortran subroutines p_iread, p_iwrit and p_wait_paraco call respectively the MPI operations: mpi_irecv, mpi_isend and mpi_waitall. The communication corresponds to a non-blocking receive with a blocking send. The BIEF_MESH structures, BUF_RECV and BUF_SEND, are declared in bief_def to receive and send the exchanged data between the sub-domains. The assembly of the sub-domain contributions in is a simple accumulation of these received data, see Listing 6.6 (line 38).

   In the compensated computation, two new structures BUF_RECV_ERR and BUF_SEND_ERR are added to also exchange the computed errors. Here the assembly is realized with the 2sum subroutine that computes the rounding error ERROR1 of the data accumulation (line 40) and ERROR2 for the error accumulation (line 42). These two values are added with the error contributions in each iteration (line 44).

Listing 6.6: The IP assembly in paraco_comp

```
! Receive step
DO IL=1,NB_NEIGHB
  IKA = NB_NEIGHB_PT(IL)
  IPA = LIST_SEND(IL)
  CALL P_IREAD(BUF_RECV(1,IL),IAN*IKA*NPLAN*8,
&              IPA,PARACO_MSG_TAG,RECV_REQ(IL))
  CALL P_IREAD(BUF_RECV_ERR(1,IL),IAN*IKA*NPLAN*8,
&              IPA,PARACO_MSG_TAG,RECV_REQ(IL))
ENDDO
! Send step
DO IL=1,NB_NEIGHB
```

```
    IKA = NB_NEIGHB_PT(IL)
    IPA = LIST_SEND(IL)
    ! Initializes the communication arrays
    K = 1
    DO J=1,NPLAN
      DO I=1,IKA
        II=NH_COM(I,IL)
        BUF_SEND(K,IL)   =V1(II,J)
        BUF_SEND_ERR(K,IL)   =ERRX(II)
        K=K+1
      ENDDO
    ENDDO
    CALL P_IWRIT(BUF_SEND(1,IL),IAN*IKA*NPLAN*8,
&                   IPA,PARACO_MSG_TAG,SEND_REQ(IL))
      CALL P_IWRIT(BUF_SEND_ERR(1,IL),IAN*IKA*NPLAN*8,
&                       IPA,PARACO_MSG_TAG,SEND_REQ(IL))
ENDDO
! Wait received messages
DO IL=1,NB_NEIGHB
    IKA = NB_NEIGHB_PT(IL)
    IPA = LIST_SEND(IL)
    CALL P_WAIT_PARACO(RECV_REQ(IL),1)
    K=1
    DO J=1,NPLAN
      DO I=1,IKA
        II=NH_COM(I,IL)
! Original version: V1(II,J)=V1(II,J)+ BUF_RECV(K,IL)
        CALL 2SUM(V1(II,J),BUF_RECV(K,IL)
    &         ,V1(II,J),ERROR1)
        CALL 2SUM(ERRV(II),BUF_RECV_ERR(K,IL)
    &         ,ERRV(II),ERROR2)
        ERROR=ERROR1+ERROR2
                ERRV(II)=ERRV(II)+ERROR
        K=K+1
      ENDDO
    ENDDO
ENDDO
```

3. The latest modification in Listing 6.4, from line 11 to 16, is the compensation after the interface point assembly. As detailed in [6], we have to compensate the accumulated errors to the data. After this step this vector becomes reproducible.

Note 3. This procedure is applied to every vector and EBE matrix. The diagonal `M%D%R` is a vector and its accompanying vector error term `M%D%E` is calculated in a similar way.

Note 4. For the studied *gouttedo* test case, the other calls of `parcom` are in the subroutines `propag, masbas2d, matrbl`. In the compensation mode, these subroutines apply the previously modifications (items 2 and 3).

6.5 Modifications in the solving phase

The resolution phase applies the conjugate gradient method provided by the subroutine `gracjg`. The modifications impact the computations of the dot product in function `p_dots`, and the EBE matrix-vector product in subroutine `matrbl`, which are called by `gracjg`.

i) The dot product $X \cdot Y$
Subroutine p_dots calls the corresponding dot product according to the computation mode, as showed in Listing 6.7.

Listing 6.7: The calls of the corresponding dot product in p_dots

```
!Declaration of a pair of double precision
 DOUBLE PRECISION PAIR(2)
!The computation of the corresponding dot product
!In the original version
!DOT for the sequential and P_DOT for parallel executions
IF (MODASS .EQ. 1) THEN
  IF(NCSIZE.LE.1.OR.NPTIR.EQ.0) THEN
    P_DOTS=DOT(NPX,X%R,Y%R)
  ELSE
    P_DOTS=P_DOT(NPX,X%R,Y%R,MESH%IFAC%I)
  ENDIF
!In the compensated version
!DOT_COMP for the sequential and P_DOTPAIR for parallel executions
ELSEIF (MODASS .EQ. 3) THEN
  IF(NCSIZE.LE.1.OR.NPTIR.EQ.0) THEN
    P_DOTS=DOT_COMP(NPX,X%R,Y%R)
  ELSE
    CALL P_DOTPAIR(NPX,X%R,Y%R,MESH%IFAC%I,PAIR)
  ENDIF
ENDIF
! Final sum on all the sub-domains (MPI subroutines)
IF (MODASS .EQ. 1) THEN
  IF(NCSIZE.GT.1) P_DOTS = P_DSUM(P_DOTS)
ELSEIF (MODASS .EQ. 3) THEN
  IF(NCSIZE.GT.1) P_DOTS = P_DSUMERR(PAIR)
ENDIF
```

In the sequential original mode (NCSIZE<1 and MODASS$=1$), the dot product is computed with the function dot as:

```
DO I = 1 , NPOIN
   DOT= DOT + X%R(I)*Y%R(I)
END DO
```

In the parallel original mode, the dot product of the whole domain is computed partially by each sub-domain, in function p_dot, as:

```
DO I = 1 , NPOIN
   P_DOT = P_DOT+X%R(I)*Y%R(I)*IFAC(I)
END DO
```

where IFAC is the weight used to avoid to compute several times the interface nodes. These partial contributions are summed over all the sub-domains to compute the global dot product by the MPI dynamic reduction in p_dsum.
In the compensated mode, a twice more accurate scalar product is computed. In sequential, function dot_comp computes a such accurate sequential dot product. It accumulates both the dot product and the generated rounding errors (addition and multiplication) and finally compensates them together.
Note: in Fortran the name of the function is the output of this function.

Listing 6.8: The sequential Dot2 in the subroutine DOT_COMP

```
CALL 2PROD(X(1),Y(1),P,EP)
```

```
DO I = 2 , NPOIN
  CALL 2PROD(X(I),Y(I),PP,EPP)
  CALL 2SUM(P,PP,P,E)
  EP=EP+(E+EPP)
END DO
DOT_COMP = P+EP
```

In the parallel implementation, each sub-domain computes its local scalar product and the corresponding generated rounding errors, to return a pair [data, error] in subroutine `p_dotpair`.

Listing 6.9: The parallel Dot2 in the subroutine `p_dotpair`

```
!Input: X(NPOIN),Y(NPOIN). Output: PAIR(2)
CALL 2PROD(X(1),Y(1)*IFAC(1),P,EP)
DO I = 2 , NPOIN
  CALL 2PROD(X(I),Y(I)*IFAC(I),PP,EPP)
  CALL 2SUM(P,PP,P,E)
  EP=EP+(E+EPP)
END DO
CALL 2SUM(P,EP,PAIR(1),PAIR(2))
```

These local pairs are exchanged between processors via MPI_ALLGATHER and are accurately accumulated by `sum2` in every processor, see Listing 6.10 in lines 8 and 11.

Listing 6.10: The final sum on all the sub-domains

```
!In original version
!CALL MPI_ALLREDUCE(MYPART,P_DSUM,1,MPI_DOUBLE_PRECISION,
!                           MPI_SUM,MPI_COMM_WORLD,IER)
!In compensated version
CALL MPI_COMM_SIZE (MPI_COMM_WORLD, NUM_PROCS, IER)
ALLOCATE(ALL_PARTIAL_SUM(1:2*NUM_PROCS))
ALL_PARTIAL_SUM=0.D0
CALL MPI_ALLGATHER (MYPART, 2, MPI_DOUBLE_PRECISION,
&                 ALL_PARTIAL_SUM,2, MPI_DOUBLE_PRECISION,
&                 MPI_COMM_WORLD, IER)
CALL SUM2(2*NUM_PROCS, ALL_PARTIAL_SUM,P_DSUMERR)
DEALLOCATE(ALL_PARTIAL_SUM)
```

ii) The matrix-vector product $M \times V$

Matrix M is stored as `M%D` of size `NPOIN` for its diagonal terms and `M%X` for its extra-diagonal ones of size `NPOIN*(NPOIN-1)` in each element `IELEM`.

The $M \times V$ product is launched by subroutine `matrbl` called in the conjugate gradient. Three subroutines are then called: `matvec`, `matvct` and `mv0303`.

In the compensated version, the subroutine parameters of the two later ones are modified to pass the associated errors `M%D%E`, `V%E`. In `mv0303`, the Hadmard product $DA \times Y$ computed by `ov_comp` is modified to update the associated errors.

Listing 6.11: EBE matrix-vector product: the multiplication of the extra-diagonal elementary terms and the diagonal terms of the matrix with the corresponding elements of the vector in `mv0303`.

```
! Here Y refers to V%R, DA refers to M%D%R and XA refers to M%X
!Contribution of extra-diagonal terms XA * Y
DO IELEM = 1 , NELEM
  W1(IELEM) = XA12(IELEM) * Y(IKLE2(IELEM))
&             + XA13(IELEM) * Y(IKLE3(IELEM))
  W2(IELEM) = XA23(IELEM) * Y(IKLE3(IELEM))
```

```
&               + XA21(IELEM) * Y(IKLE1(IELEM))
  W3(IELEM) = XA31(IELEM) * Y(IKLE1(IELEM))
&               + XA32(IELEM) * Y(IKLE2(IELEM))
END DO
!Contribution of the diagonal DA * Y
IF ( MODASS .EQ.1) THEN
  CALL OV ('X=YZ    ', X , Y , DA , C  , NPOIN )
ELSEIF (MODASS .EQ. 3) THEN
  CALL OV_COMP ('X=YZ    ', X , Y , DA , C  , NPOIN
 &              ,X_ERR, Y_ERR , DA_ERR   )
ENDIF
```

Listing 6.11 (from lines 3 to 10) illustrates the process of the elementary contribution computations. These latter proceed to a finite element assembly. In the compensation mode, this assembly is performed as we detailed in subroutine assvec (Listing 6.5). The final step assembles the matrix-vector product at the interface point in matrbl with a parcom call and finishes with a compensation operations.

6.6 Conclusion

In this chapter we detail, with a technical point of view, the modifications we introduced in openTelemac to recover the reproducibility of the studied test cases. The first difficulty in this work was to define and to apply the methodology detailed in Section 6.1 to such a huge code. The second difficulty was to identify the sources of non-reproducibility, *i.e.* where the rounding errors differ between the sequential and the parallel simulations, and to distinguish their implementations in (again) this huge code. It was inevitable to manipulate three openTelemac components: the BIEF library, the parallel library and Telemac-2D module which include respectively 493, 46 and 192 subroutines. The modifications to obtain reproducibility were restricted to about 30 subroutines, mostly in BIEF. We list these modified subroutines at the end of this section.
The first source is the non-deterministic error propagation at the interfaces nodes. We recall again that this step is implicitly present in several parts of the computation (building and solving phases). It is sufficient to store and propagate these errors and finally to compensate them into the computed value after every step of interface node assembly. These corrections are applied for both the parallel and the sequential simulations to yield the expected reproducibility between the two execution modes. The second source is the dynamic reduction of the parallel implementation for the dot product in the conjugate gradient iterations. It is corrected by implementing a dot product that computes in about twice the working precision. Here it yields reproducible results whereas this is not true for very ill-conditioned ones. In this latter case, more compensated steps can be applied for instance.

We think that these details are important to the continuity of this work. Of course, that this chapter necessitates a little knowing of openTelemac code. The integration of our modifications is still in progress and it is expected that this will be available in the next distributed version of openTelemac. One integration difficulty is that the code was changed in the meantime of this work, which requires a careful merge between all these modifications.

List of modified subroutines

BIEF library.

- ***Modified:*** almesh, assvec, bief, bief_allvec, bief_def, matrbl, matrix, matvec, om, mv_0303, om_1111, os, p_dots, parini, precd1, solve, vectos.

- ***Added:*** `ov_comp`, `dot_comp`, `p_dot_comp`, `parcom_comp`, `parcom2_comp`, `paraco_comp`,`twosum`, `twoprod`.

Parallel library.

- ***Modified:*** `interface_parallel`.
- ***Added:*** `p_dsum_err`.

Telemac-2D module.

- ***Modified:*** `lecdon_telemac`, `masbas2d`, `propag`, `telemac2d.dico`.

7. Development life in Telemac

Greetings fellow TELEMAC-MASCARET SYSTEM developer and welcome into the world of a TELEMAC-MASCARET SYSTEM developer. It might be hard at the beginning but with time you will unravel all of TELEMAC-MASCARET SYSTEM dirty little secrets. This Guide aims to describe all the steps you might encounter when developing in TELEMAC-MASCARET SYSTEM, those steps can be found in the "TELEMAC-MASCARET SYSTEM Software Qualtiy Plan" (Eureka H-P74-2014-02365-EN). They are resumed in the Fig 7.1.

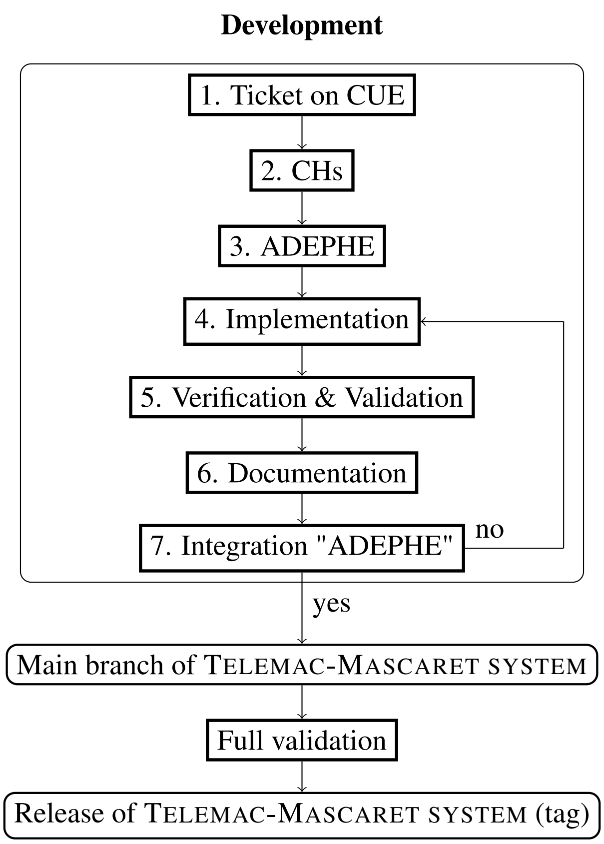


Figure 7.1: Life cycle of a TELEMAC-MASCARET SYSTEM development

The following sections will describes how to use the three tools you will be using during your development:

- SVN, The source controller that you will be using to handle the sources of your development.
- CUE, The ticket manager which will contain information on your development.
- CIS, The Continuous Integration Service which will compile, run, and validation your developments.

7.1 Information to give when your development is beginning

To begin you work you will need to send an email to `awe@hrwallingford.com` with the following informations in order to give you the proper access into the TELEMAC-MASCARET SYSTEM developing world:

- Your Name.
- The name of a fish (for the SVN branch, any existing fish is okay).
- The TELEMAC-MASCARET SYSTEM modules on which you will be working (See Section 10.1).
- The demand to add your branch on CIS.

7.2 Information to give when your development is over

This section will give a list of all the information you need to give to the person in charge of the integration of your development.

- CUE ticket number.
- Name of the branch the work is done on.
- Revision range of work I.e. The revision number of when you started your development and when it ended on your SVN branch.
- A list of the file impacted by the development (See 11.6 on how to create that list).
- The name of the test cases validating the development (17.2 on how to add a new test case).

All those information should be written in the CUE ticket as well.

8. TELEMAC-MASCARET SYSTEM Coding Convention

8.1 Main rules

We give hereafter a number of safety rules that will avoid most common disasters. It is however highly recommended to THINK before implementing. The structure of your code and the choice of the algorithms will deeply influence: the manpower requested, the number of lines to write, the memory requested, the computer time. For a given task, differences of a factor 10 for these 4 items are common and have been documented (see e.g. "the mythical man-month, essays on software engineering" by Frederick Brooks). These differences will eventually result in "success" or "failure". So let the power be with you and just follow Yoda's advice: "when you look at the dark side, careful you must be".

8.2 Subroutine header

```
!                        ****************
                         SUBROUTINE METEO
!                        ****************
!
     &(PATMOS,WINDX,WINDY,FUAIR,FVAIR,X,Y,AT,LT,NPOIN,VENT,ATMOS,
     & HN,TRA01,GRAV,ROEAU,NORD,PRIVE)
!
!***********************************************************************
! TELEMAC2D   V6P2                                   27/07/2012
!***********************************************************************
!
!brief    COMPUTES ATMOSPHERIC PRESSURE AND WIND VELOCITY FIELDS
!+                (IN GENERAL FROM INPUT DATA FILES).
!
!warning  MUST BE ADAPTED BY USER
!
!history  J-M HERVOUET (LNHE)
!+        02/01/2004
!+        V5P4
!+
!
```

```
!history  N.DURAND (HRW), S.E.BOURBAN (HRW)
!+        13/07/2010
!+        V6P0
!+   Translation of French comments within the FORTRAN sources into
!+   English comments
!
!history  N.DURAND (HRW), S.E.BOURBAN (HRW)
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!+        V6P0
!+   Creation of DOXYGEN tags for automated documentation and
!+   cross-referencing of the FORTRAN sources
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| AT,LT          |-->| TIME, ITERATION NUMBER
!| ATMOS          |-->| YES IF PRESSURE TAKEN INTO ACCOUNT
!| FUAIR          |-->| VELOCITY OF WIND ALONG X, IF CONSTANT
!| FVAIR          |-->| VELOCITY OF WIND ALONG Y, IF CONSTANT
!| GRAV           |-->| GRAVITY ACCELERATION
!| HN             |-->| DEPTH
!| NORD           |-->| DIRECTION OF NORTH, COUNTER-CLOCK-WISE
!|                |   | STARTING FROM VERTICAL AXIS
!| NPOIN          |-->| NUMBER OF POINTS IN THE MESH
!| PATMOS         |<--| ATMOSPHERIC PRESSURE
!| PRIVE          |-->| USER WORKING ARRAYS (BIEF_OBJ BLOCK)
!| ROEAU          |-->| WATER DENSITY
!| TRA01          |-->| WORKING ARRAY
!| VENT           |-->| YES IF WIND TAKEN INTO ACCOUNT
!| WINDX          |<--| FIRST COMPONENT OF WIND VELOCITY
!| WINDY          |<--| SECOND COMPONENT OF WIND VELOCITY
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
      USE BIEF
!
      IMPLICIT NONE
      INTEGER LNG,LU
      COMMON/INFO/LNG,LU
!
!+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+
!
      INTEGER, INTENT(IN)                   :: LT,NPOIN
      LOGICAL, INTENT(IN)                   :: ATMOS,VENT
      DOUBLE PRECISION, INTENT(IN)          :: X(NPOIN),Y(NPOIN),HN(NPOIN)
      DOUBLE PRECISION, INTENT(INOUT)       :: WINDX(NPOIN),WINDY(NPOIN)
      DOUBLE PRECISION, INTENT(INOUT)       :: PATMOS(NPOIN),TRA01(NPOIN)
      DOUBLE PRECISION, INTENT(IN)          :: FUAIR,FVAIR,AT,GRAV,ROEAU,NORD
      TYPE(BIEF_OBJ), INTENT(INOUT)         :: PRIVE
!
!+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+
!
```

```
!       LOCAL DECLARATIONS
!
        DOUBLE PRECISION P0,Z(1)
!
```

8.3 The coding convention

- The code must pass Fortran 2003 Standard,
- A file must contain only one program/module/subroutine/function and must have the same name as that program/module/subroutine/function,
- The extension of the file should be ".F" if it contains preprocessing commands to control access to an external library. This is the case for the files in the parrallel module.
- All subroutines and functions must conform to the subroutine header given in the previous paragraph,
- All subroutines and functions must be protected by an IMPLICIT NONE statement. Their arguments types must be given with their INTENT,
- The order in declarations is free except than some compilers will not accept that an array has a dimension that has not been declared before, hence:

  ```
  INTEGER, INTENT(IN) :: N
  DOUBLE PRECISION, INTENT(INOUT) :: DEPTH(N)
  ```

  is correct and:

  ```
  DOUBLE PRECISION, INTENT(INOUT) :: DEPTH(N)
  INTEGER, INTENT(IN) :: N
  ```

  is not correct.
- Error messages: they must be given in French and English, using logical unit LU taken in COMMON block INFO. LNG = 1 is French, LNG = 2 is English. Parameterizing the listing logical unit is necessary because it is not always 6 in parallel, as the listing of slave processors does not appear on the screen but is redirected to files.
- Lines must be limited to a size of 72 characters, and only in UPPERCASE. Spaces must be only one blank, for example between a CALL and the name of a subroutine. This is to facilitate research of character string in source code,
- Indents in IF statements and nested loops are of 2 blanks,
- Tabs for indenting are forbidden. The reason is that depending on compilers they represent a random number of blanks (6, 8, etc.) and that it is not standard Fortran,
- Blank lines are better started by a “!”.
- Comments line should begin with a "!".
- Names of variables: a name of variable should not be that of an intrinsic function, e.g. do not choose names like MIN, MAX, MOD, etc., though possible in theory this may create conflicts in some compilers, for example the future Automatic Differentiation Nag compiler.

- Functions: intrinsic functions must be declared as such. Use only the generic form of intrinsic functions, e.g. MAX(1.D0,2.D0) and not DMAX(1.D0,2.D0). It is actually the generic function MAX that will call the function DMAX in view of your arguments, you are not supposed to do the job of the compiler.

8.4 Defensive programming

When programming, one has always to keep in mind that wrong information may have been given by the user, or that some memory fault has corrupted the data. Hence when an integer OPT may only have 2 values, say 1 and 2 for option 1 and option 2, always organise the tests as follows:

```
IF(OPT.EQ.1) THEN
  ! here option 1 is applied
ELSEIF(OPT.EQ.2) THEN
  ! here option 2 is applied
ELSE
  ! here something wrong happened, it is dangerous to go further, we stop.
  IF(LNG.EQ.1) THEN
    WRITE(LU,*) 'OPT=',OPT,' OPTION INCONNUE DANS LE SOUS-PROGRAMME...'
  ENDIF
  IF(LNG.EQ.2) THEN
    WRITE(LU,*) 'OPT=',OPT,' IS AN UNKNOWN OPTION IN SUBROUTINE...'
  ENDIF
  CALL PLANTE(1)
  STOP
ENDIF
```

8.5 Over-use of modules

Modules are very useful but used in excess, they may become very tricky to handle without recompiling the whole libraries. For example the declaration modules containing all the global data of a program cannot be changed without recompiling all subroutines that use it.
A common way of developing software in the TELEMAC-MASCARET SYSTEM system is to add modified subroutines in the user FORTRAN FILE. This will sometimes be precluded for modules as some conflicts with already compiled modules in libraries will appear.
A moderate use of modules is thus prescribed (though a number of inner subroutines in BIEF would deserve inclusion in modules).

8.6 Allocating memory

For optimisation no important array should be allocated at every time step, it is better to use the work arrays allocated once for all in TELEMAC-MASCARET SYSTEM programs, like $T1$, $T2$, etc., in TELEMAC-2D (note that they are $BIEF_OBJ$ structures, which brings some protection against misuses). If it cannot be avoided, an array allocated locally should be clearly visible and:

- Either allocated once and declared with a command SAVE,

- Or if used once only, deallocated at the end of the subroutine.

Automatic arrays are strictly forbidden. For example the array X in the following line:

```
DOUBLE PRECISION X(NPOIN)
```

If it is not in the subroutine arguments, while $NPOIN$ is. In this case it is a hidden allocation of size $NPOIN$, which may change from one call to the other. It is not standard Fortran, in worst cases it will cause a compiler to crash after a number of calls..

8.7 Test on small numbers

Always think that computers do truncation errors. Tests like: $IF(X.EQ.0.D0)THEN\ldots$ are very risky if X is the result of a computation. Allow some tolerance, like: $IF(ABS(X).LT.1.D-10)THEN\ldots$, especially if divisions are involved.

8.8 Optimisation

Optimisation is a key point, a badly written subroutine may spoil the efficiency of the whole program. Optimisation is a science and even an art, but it can be interesting to have a few ideas or tricks in mind. Here are a few examples:
Example 1: powers
The following loop:

```
DO I=1,NPOIN
  X(I)=Y(I)**2.D0
ENDDO
```

is a stupid thing to do and should be replaced by:

```
DO I=1,NPOIN
  X(I)=Y(I)**2
ENDDO
```

As a matter of fact, $Y(I)**2$ is a single multiplication, $Y(I)**2.D0$ is an exponential ($exp(2.D0*Log(Y))$), it costs a lot, and moreover will crash if $Y(I)$ negative.
Example 2: intensive loops with useless tests
Case 1: the following loop

```
DO I=1,NPOIN
   IF(OPTION.EQ.1) THEN
     X(I)=Y(I)+2.D0
  ELSE
    X(I)=Y(I)+Z(I)
  ENDIF
ENDDO
```

Should be replaced by:

```
IF(OPTION.EQ.1) THEN
  DO I=1,NPOIN
    X(I)=Y(I)+2.D0
  ENDDO
ELSE
DO I=1,NPOIN
```

```
      X(I)=Y(I)+Z(I)
   ENDDO
ENDIF
```

In the first case the test on $OPTION$ is done $NPOIN$ times, in the latter it is done once.
Case 2: the following loop

```
DO I=1,NPOIN
      IF(Z(I).NE.0.D0) X(I)=X(I)+Z(I)
ENDDO
```

seems a good idea to avoid doing useless additions, but forces a lot of tests and actually spoils computer time, prefer:

```
DO I=1,NPOIN
      X(I)=X(I)+Z(I)
ENDDO
```

Example 3: strides
Declaring an array as $XM(NELEM,30)$ or $XM(30,NELEM)$ for storing 30 values per element is not innocent with respect to optimisation. The principle in Fortran is that in memory the first index varies first. If you want to sum values number 15 of all elements, the first declaration is more appropriate. If you want to sum the 30 values of element 1200 the second declaration is more appropriate. The principle is that the values that are summed should be side by side in the memory.
A lot remains to be done in TELEMAC-MASCARET SYSTEM on strides. Sometimes it brings an impressive optimisation (case of murd3d.f in library TELEMAC-3D, with XM declared as $XM(30,NELEM)$ unlike the usual habit), sometimes it makes no change, e.g. the matrix-vector product in segments seems to be insensitive to the declaration of $GLOSEG$ as $(NSEG,2)$ or $(2,NSEG)$. This can be compiler dependent.
Example 4: the use and abuse of subroutine OS
Using subroutine OS is meant for simple operations like $X(I) = Y(I) + Z(I)$. Do not combine long lists of successive calls of OS to compute a complex formula, do it in a simple loop.
Thus the following sequence taken from bedload_seccurrent.f in SISYPHE:

```
CALL OS('X=YZ     ', X=T2, Y=QU, Z=QU) ! QU**2
CALL OS('X=Y/Z    ', X=T2, Y=T2, Z=HN) ! QU**2/HN
CALL OS('X=Y/Z    ', X=T2, Y=T2, Z=HN) ! QU**2/HN**2
CALL OS('X=YZ     ', X=T3, Y=QV, Z=QV) ! QV**2
CALL OS('X=Y/Z    ', X=T3, Y=T3, Z=HN) ! QV**2/HN
CALL OS('X=Y/Z    ', X=T3, Y=T3, Z=HN) ! QV**2/HN**2
CALL OS('X=X+Y    ', X=T2, Y=T3)       ! QU**2+QV**2/HN**2
```

should be better written (once the discretization of $T2$ is secured, for example by $CALL\ CPSTVC(QU,T2)$):

```
DO I=1,NPOIN
   T2%R(I)=(QU%R(I)**2+QV%R(I)**2)/HN%R(I)**2
ENDDO
```

8.9 Parallelism and tidal flats

Parallelism and tidal flats are VERY demanding for algorithms. For example parallelism often doubles the time of development. It is also the case of tidal flats that bring many opportunities of divisions by zero and a number of extra problems. New algorithms must then be duly tested against parallelism and tidal flats or, in 3D, cases where elements are crushed.

8.10 Adding a new output variable

In most of the modules you can find the keyword `VARIABLES FOR GRAPHIC PRINTOUTS` or something alike. This defines the variable to write in the module output file. Here we will describe what need to be done to add a new one. The example below is made for telemac2d but all the modules follow the same behaviour.
To be added to the output variables the variable must validate the followin points:

- It must be stored in a bief_obj.
- It must be disctretized on the number of points.

- Add the variable in the dictionary for the keywords for graphical and listing outputes. Add them in both CHOIX and CHOIX1. Also do not forget to add them in AIDE and AIDE1 as well. The short name of the variable must not exceed 8 characters. The short name must also be the name of the bief_obj containing the variable.
- Add the variable to the bief_obj varsor (in TELEMAC-3D varsor is for 2d output varso3 is for 3d output) in `point_telemac2d.f`.
- Add the variable names and unit in TEXT and TEXTPR in `nomvar_telemac2d.f`. Also fill the mnemo with the short name you used in the ditionary. Increase the variable NVAR_T2D.

9. Hermes

9.1 Description

The aim of this module is to produce generic functions to read/write meshes, data and boundary conditions in TELEMAC-MASCARET SYSTEM regardless of the file format. For that purpose a new module, called Hermes, was created.

9.2 User Manual

Three formats are now available in TELEMAC-MASCARET SYSTEM:

- SERAFIN, TELEMAC-MASCARET SYSTEM own format, a binary containing the mesh and the results information, all the real are in single precision.
- SERAFIND, same as above but the real are in double precision.
- MED, a binary format based on hdf5, format used by the Salome platform. This format requires to install additional libraries and add specific option to the TELEMAC-MASCARET SYSTEM installation therefore it not installed by default.

In order to set the file format, a keyword is defined for every file, for example the keyword for "geometry file" is "geometry file format".
All the files used for a simulation must be in the same format, this is due to the fact that the same boundary file is used for all the files and the boundary file is format-dependant. Only SERAFIN an SERAFIND can coexist as they are using the same format for their boundary file.

9.2.1 List of functions

Mesh functions

```
subroutine open_mesh(fformat,file_name,file_id,openmode,ierr)
!
!brief    opens a mesh file
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| file_name      |-->| name of the file
!| file_id        |-->| file descriptor
```

```
!| openmode       |-->| one of the following value 'read','write','readwrite'
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
  character(len=8),  intent(in)    :: fformat
  character(len=*), intent(in)   :: file_name
  integer,           intent(in)   :: file_id
  character(len=9), intent(in)     :: openmode
  integer, intent(out)             :: ierr
!
end subroutine
```

```
subroutine close_mesh (fformat,file_id,ierr)
!
!brief    closes a mesh file
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| file_id        |-->| file descriptor
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
  character(len=8),  intent(in)    :: fformat
  integer,           intent(in)   :: file_id
  integer, intent(out)             :: ierr
!
end subroutine
```

```
subroutine get_mesh_title (fformat,fid,title,ierr)
!
!brief    returns the title from a mesh file
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| title          |<->| title of the mesh file
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8),  intent(in)  :: fformat
  integer,           intent(in)  :: fid
  character(len=80), intent(inout) :: title
  integer,           intent(out) :: ierr
!
end subroutine
```

```
subroutine get_mesh_date (fformat,fid,date,ierr)
!
!brief    returns the date of the mesh file
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
```

```
!| fid             |-->| file descriptor
!| date            |<->| the date
!| ierr            |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)   :: fformat
  integer,          intent(in)   :: fid
  integer,          intent(inout) :: date(6)
  integer,          intent(out)  :: ierr
!
end subroutine
```

```
subroutine get_mesh_nelem (fformat,fid,typ_elem,nelem,ierr)
!
!brief    returns the number of elements of type typ_elem in the mesh file
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat         |-->| format of the file
!| fid             |-->| file descriptor
!| typ_elem        |-->| type of the element
!| nelem           |<->| the number of elements
!| ierr            |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)   :: fformat
  integer,          intent(in)   :: fid
  integer,          intent(in)   :: typ_elem
  integer,          intent(inout) :: nelem
  integer,          intent(out)  :: ierr
!
end subroutine
```

```
subroutine get_mesh_ndp (fformat,fid,typ_elem,ndp,ierr)
!
!brief    returns the number of point per element of type typ_elem
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat         |-->| format of the file
!| fid             |-->| file descriptor
!| typ_elem        |-->| type of the element
!| ndp             |<->| the number of point per element
!| ierr            |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)   :: fformat
  integer,          intent(in)   :: fid
  integer,          intent(in)   :: typ_elem
  integer,          intent(inout) :: ndp
  integer,          intent(out)  :: ierr
!
```

```
end subroutine
```

```
subroutine get_mesh_ikle (fformat,fid,typ_elem,ikle,nelem,ndp,ierr)
!
!brief    returns the connectivity table for
!+        the element of type typ_elem in the mesh
!+        will do nothing if there are no element of typ_elem in the mesh
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| typ_elem       |-->| type of the element
!| ikle           |<->| the connectivity table
!| nelem          |-->| number of elements
!| ndp            |-->| number of points per element
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)   :: fformat
  integer,          intent(in)   :: fid
  integer,          intent(in)   :: typ_elem
  integer,          intent(in)   :: nelem
  integer,          intent(in)   :: ndp
  integer,          intent(inout) :: ikle(nelem*ndp)
  integer,          intent(out)  :: ierr
!
end subroutine
```

```
subroutine get_mesh_npoin (fformat,fid,typ_elem,npoin,ierr)
!
!brief    returns the number of point for the given element type in the mesh
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| typ_elem       |-->| type of the element
!| npoin          |<->| the number of points
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)   :: fformat
  integer,          intent(in)   :: fid
  integer,          intent(in)   :: typ_elem
  integer,          intent(inout) :: npoin
  integer,          intent(out)  :: ierr
!
end subroutine
```

```
subroutine get_mesh_nplan (fformat,fid,nplan,ierr)
!
```

```
!brief    returns the number of layers
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| nplan          |<->| the number of layers
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: fid
  integer,          intent(inout) :: nplan
  integer,          intent(out) :: ierr
!
end subroutine
```

```
subroutine get_mesh_dimension (fformat,fid,ndim,ierr)
!
!brief    returns the number of dimensions of the space
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| ndim           |<->| number of dimension
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: fid
  integer,          intent(inout) :: ndim
  integer,          intent(out) :: ierr
!
end subroutine
```

```
subroutine get_mesh_coord (fformat,fid,jdim,ndim,npoin,coord,ierr)
!
!brief    returns the coordinates for the given dimension
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| jdim           |-->| dimension number
!| ndim           |-->| number of dimension of the mesh
!| npoin          |-->| total number of nodes
!| coord          |<->| local to global numbering array
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: fid, jdim, ndim, npoin
```

```
  double precision, intent(inout) :: coord(npoin)
  integer,          intent(out) :: ierr
!
end subroutine
```

```
subroutine get_mesh_knolg (fformat,fid,knolg,npoin,ierr)
!
!brief    returns the local to global numbering array
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| knolg          |<->| local to global numbering array
!| npoin          |-->| number of nodes
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: fid
  integer,          intent(in)  :: npoin
  integer,          intent(inout) :: knolg(npoin)
  integer,          intent(out) :: ierr
!
end subroutine
```

```
subroutine get_mesh_nptir (fformat,fid,nptir,ierr)
!
!brief    returns the number of interface point
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| nptir          |<->| number of interface point
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: fid
  integer,          intent(inout) :: nptir
  integer,          intent(out) :: ierr
!
end subroutine
```

Boundary functions

```
subroutine open_bnd(fformat,file_name,file_id,openmode,ierr)
!
!brief    opens a boundary file
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
```

```
!| file_name      |-->| name of the file
!| file_id        |-->| file descriptor of the "mesh" file
!| openmode       |-->| one of the following value 'read','write','readwrite'
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
  character(len=8),  intent(in)    :: fformat
  character(len=*), intent(in)   :: file_name
  integer,           intent(in)   :: file_id
  character(len=9), intent(in)    :: openmode
  integer, intent(out)            :: ierr
!
end subroutine
```

```
subroutine close_bnd (fformat,file_id,ierr)
!
!brief    closes a boundary file
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| file_id        |-->| file descriptor of the "mesh" file
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
  character(len=8),  intent(in)    :: fformat
  integer,           intent(in)   :: file_id
  integer, intent(out)            :: ierr
!
end subroutine
```

```
subroutine get_bnd_ipobo (fformat,fid,npoin,nelebd,typ_bnd_elem,ipobo,ierr)
!
!brief    returns an array containing
!+        1 if a point is a boundary point 0 otherwise
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| npoin          |-->| total number of nodes
!| nelebd         |-->| total number of boundary elements
!| typ_bnd_elem   |-->| type of the boundary element
!| ipobo          |<->| an array containing
!|                |   | 1 if a point is a boundary point 0 otherwise
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: fid, npoin, nelebd, typ_bnd_elem
  integer,          intent(inout) :: ipobo(npoin)
  integer,          intent(out) :: ierr
!
end subroutine
```

```
subroutine get_bnd_nbor (fformat,fid,typ_bnd_elem,nptfr,nbor,ierr)
!
!brief    returns an array containing
!+        the association of boundary numbering to mesh numbering
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| typ_bnd_elem   |-->| type of the boundary element
!| nptfr          |-->| number of boundary points
!| nbor           |<->| an array containing the numbering in the mesh
!|                |   | of all boundary points
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: fid, nptfr, typ_bnd_elem
  integer,          intent(inout) :: nbor(nptfr)
  integer,          intent(out) :: ierr
!
end subroutine
```

```
subroutine get_bnd_ikle (fformat,fid,typ_bnd_elem,nelebd,ndp,ikle_bnd,ierr)
!
!brief    reads the connectivity of the boundary elements
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| typ_bnd_elem   |-->| type of the boundary elements
!| nelebd         |-->| number of boundary elements
!| ndp            |-->| number of points per element
!| ikle_bnd       |<->| the connectivity of the boundary elements
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in) :: fformat
  integer, intent(in) :: fid,typ_bnd_elem,nelebd,ndp
  integer, intent(inout) :: ikle_bnd(ndp*nelebd)
  integer, intent(out) :: ierr
!
end subroutine
```

```
subroutine get_bnd_npoin (fformat,fid,type_bnd_elem,nptfr,ierr)
!
!brief    returns the number of boundary points
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
```

```
!| type_bnd_elem  |-->| type of the boundary elements
!| nptfr          |<->| number of boundary points
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: fid
  integer,          intent(in)  :: type_bnd_elem
  integer,          intent(inout) :: nptfr
  integer,          intent(out) :: ierr
!
end subroutine
```

```
subroutine get_bnd_nelem (fformat,fid,type_bnd_elem,nelem,ierr)
!
!brief    reads the number of boundary elements
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| type_bnd_elem  |-->| type of the boundary elements
!| nelem          |<->| number of boundary elements
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: fid
  integer,          intent(in)  :: type_bnd_elem
  integer,          intent(inout) :: nelem
  integer,          intent(out) :: ierr
!
end subroutine
```

```
subroutine get_bnd_value (fformat,fid,typ_bnd_elem,nelebd,value,nptfr,nbor,ie
!
!brief    returns an array containing the boundary type for each boundary poi
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| typ_bnd_elem   |-->| type of the boundary elements
!| nelebd         |-->| number of boundary elements
!| value          |<->| type of boundary for each point
!| nptfr          |-->| number of boundary points
!| nbor           |-->| boundary to global numbering array
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: fid
```

```
  integer,          intent(in)   :: typ_bnd_elem
  integer,          intent(in)   :: nelebd
  integer,          intent(in)   :: nptfr
  integer,          intent(inout) :: value(nptfr)
  integer,          intent(in) :: nbor(nptfr)
  integer,          intent(out) :: ierr
!
end subroutine
```

Data functions

```
subroutine get_data_nvar (fformat,fid,nvar,ierr)
!
!brief    returns the number of variables in the mesh file
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| nvar           |<->| number of variable
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)   :: fformat
  integer,          intent(in)   :: fid
  integer,          intent(inout) :: nvar
  integer,          intent(out) :: ierr
!
end subroutine
```

```
subroutine get_data_var_list (fformat,fid,nvar,varlist,unitlist,ierr)
!
!brief    returns a list of all the name of the variables in the mesh file
!+        and a list of their units
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| varlist        |<->| list of variable name
!| untilist       |<->| list of variable unit
!| ierr           |<--| 0 if no error during the execution
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8),  intent(in)   :: fformat
  integer,           intent(in)   :: fid
  integer,           intent(in)   :: nvar
  character(len=16), intent(inout) :: varlist(nvar)
  character(len=16), intent(inout) :: unitlist(nvar)
  integer,           intent(out) :: ierr
!
end subroutine
```

```
subroutine get_data_ntimestep (fformat,fid,ntimestep,ierr)
!
!brief    returns the number of time step in the mesh file
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| ntimestep      |<->| the number of time steps
!| ierr           |<--| 0 if no error during the execution
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: fid
  integer,          intent(inout) :: ntimestep
  integer,          intent(out) :: ierr
!
end subroutine
```

```
subroutine get_data_time (fformat,fid,record,time,ierr)
!
!brief    returns the time value of a given time step
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| record         |-->| number of the time step
!| time           |<->| time in second of the time step
!| ierr           |<--| 0 if no error during the execution
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: fid
  integer,          intent(in)  :: record
  double precision, intent(inout) :: time
  integer,          intent(out) :: ierr
!
end subroutine
```

```
subroutine get_data_value (fformat,fid,record,var_name,res_value,n,ierr)
!
!brief    returns the value for each point of a given variable
!+        for a given time step
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| file_id        |-->| file descriptor
!| record         |-->| time step to read in the file
!| var_name       |-->| variable for which we need the value
!| res_value      |<->| value for each point at time step record
!|                |   | for the variable var_name
```

```
!| n                |-->| size of res_value
!| ierr             |<--| 0 if no error during the execution
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8),  intent(in)    :: fformat
  integer,           intent(in)    :: fid
  integer,           intent(in)    :: record
  character(len=16), intent(in)    :: var_name
  integer,           intent(in)    :: n
  double precision,  intent(inout) :: res_value(n)
  integer,           intent(out)   :: ierr
!
end subroutine
```

Writing functions

```
subroutine set_header (fformat,file_id,title,nvar,var_name,ierr)
!
!brief    writes the title and the name and units of the variables
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat          |-->| format of the file
!| file_id          |-->| file descriptor
!| title            |-->| title of the mesh
!| nvar             |-->| number of variables
!| var_name         |-->| name and units of the variables
!| ierr             |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8),  intent(in)  :: fformat
  integer,           intent(in)  :: file_id
  character(len=80), intent(in)  :: title
  integer,           intent(in)  :: nvar
  character(len=32), intent(in)  :: var_name(nvar)
  integer,           intent(out) :: ierr
!
end subroutine
```

```
subroutine set_mesh
    (fformat,file_id,mesh_dim,typelm,ndp,nptfr,
     nptir,nelem,npoin,ikle,ipobo,
     knolg,x,y,nplan,date,time,ierr,z)
!
!brief    writes the mesh geometry in the file
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat          |-->| format of the file
!| file_id          |-->| file descriptor
!| mesh_dim         |-->| dimension of the mesh
!| typelm           |-->| type of the mesh elements
!| ndp              |-->| number of points per element
```

```
!| nptfr          |-->| number of boundary point
!| nptir          |-->| number of interface point
!| nelem          |-->| number of element in the mesh
!| npoin          |-->| number of points in the mesh
!| ikle           |-->| connectivity array for the main element
!| ipobo          |-->| is a boundary point ? array
!| knolg          |-->| local to global numbering array
!| x              |-->| x coordinates of the mesh points
!| y              |-->| y coordinates of the mesh points
!| nplan          |-->| number of planes
!| date           |-->| date of the creation of the mesh
!| time           |-->| time of the creation of the mesh
!| ierr           |<--| 0 if no error during the opening
!| z  (optional)  |-->| z coordinates of the mesh points
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: file_id,nplan
  integer,          intent(in)  :: date(3)
  integer,          intent(in)  :: time(3)
  integer,          intent(in)  :: mesh_dim
  integer,          intent(in)  :: typelm
  integer,          intent(in)  :: ndp
  integer,          intent(in)  :: nptfr
  integer,          intent(in)  :: nptir
  integer,          intent(in)  :: nelem
  integer,          intent(in)  :: npoin
  integer,          intent(in)  :: ikle(nelem*ndp)
  integer,          intent(in)  :: ipobo(npoin)
  integer,          intent(in)  :: knolg(npoin)
  double precision, intent(in)  :: x(npoin),y(npoin)
  integer,          intent(out) :: ierr
  double precision, intent(in), optional :: z(npoin)
!
end subroutine
```

```
subroutine set_bnd (fformat,fid,type_bnd_elt,nelebd,ndp,ikle,value,ierr)
!
!brief    writes the boundary information into the mesh file
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| fid            |-->| file descriptor
!| type_bnd_elt   |-->| type of the boundary elements
!| nelebd         |-->| number of boundary elements
!| ndp            |-->| number of points per boundary element
!| ikle           |-->| connectivity array for the boundary elements
!| value          |-->| value for each boundary element
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
```

```
!
  character(len=8), intent(in)  :: fformat
  integer,          intent(in)  :: fid
  integer,          intent(in)  :: type_bnd_elt
  integer,          intent(in)  :: nelebd
  integer,          intent(in)  :: ndp
  integer,          intent(in)  :: ikle(nelebd*ndp)
  integer,          intent(in)  :: value(nelebd)
  integer,          intent(out) :: ierr
!
end subroutine
```

```
subroutine add_data
     (fformat,file_id,var_name,time,record,
      first_var,var_value,n,ierr)
!
!brief    add data information for a given variable and a given time on
!+        all points of the mesh
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| fformat        |-->| format of the file
!| file_id        |-->| file descriptor
!| var_name       |-->| name of the variable
!| time           |-->| time of the data
!| record         |-->| time step of the data
!| first_var      |-->| true if it is the first variable of the dataset
!| var_value      |-->| the value for each point of the mesh
!| n              |-->| size of var_value
!| ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
      character(len=8),  intent(in)  :: fformat
      integer,           intent(in)  :: file_id,n
      character(len=32), intent(in)  :: var_name
      double precision,  intent(in)  :: time
      integer,           intent(in)  :: record
      logical,           intent(in)  :: first_var
      double precision,  intent(in)  :: var_value(n)
      integer,           intent(out) :: ierr
!
end subroutine
```

9.3 Developer Manual

9.3.1 Structure of the module

The module is divided into three parts:

- The file `interface_hermes.f` which contains the list of the reading/writing functions.
- A file for each of the function listed in `interface_hermes.f`.

- A module for each format handled in TELEMAC-MASCARET SYSTEM.

All the files of the second part look more or less like this:

```
!                    *******************
                     SUBROUTINE OPEN_MESH
!                    *******************
!
     &(FFORMAT,FILE_NAME,FILE_ID,OPENMODE,IERR)
!
!***********************************************************************
! HERMES   V7P0                                               01/05/2014
!***********************************************************************
!
!brief    OPENS A MESH FILE
!
!history  Y AUDOUIN (LNHE)
!+        24/03/2014
!+        V7P0
!+
!
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!| FFORMAT        |-->| FORMAT OF THE FILE
!| FILE_NAME      |-->| Name of the file
!| FILE_ID        |-->| File descriptor
!| OPENMODE       |-->| ONE OF THE FOLLOWING VALUE 'READ','WRITE','READWRITE'
!| Ierr           |<--| 0 if no error during the opening
!~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
!
      USE UTILS_SERAFIN
      USE UTILS_MED
      IMPLICIT NONE
      INTEGER     LNG,LU
      COMMON/INFO/LNG,LU
!
!+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+
!
      CHARACTER(LEN=8),  INTENT(IN)     :: FFORMAT
      CHARACTER(LEN=*), INTENT(IN)     :: FILE_NAME
      INTEGER,            INTENT(IN)     :: FILE_ID
      CHARACTER(LEN=9), INTENT(IN)      :: OPENMODE
      INTEGER, INTENT(OUT)              :: IERR
!
!+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+-+
!
      SELECT CASE (FFORMAT)
        CASE ('SERAFIN ','SERAFIND')
          CALL OPEN_MESH_SRF(FILE_NAME, FILE_ID, OPENMODE,FFORMAT, IERR)
        CASE ('MED     ')
          CALL OPEN_MESH_MED(FILE_NAME, FILE_ID, OPENMODE,IERR)
        CASE DEFAULT
```

```
          IF(LNG.EQ.1) THEN
            WRITE(LU,*) 'OPEN_MESH : MAUVAIS FORMAT : ',FFORMAT
          ENDIF
          IF(LNG.EQ.2) THEN
            WRITE(LU,*) 'OPEN_MESH: BAD FILE FORMAT: ',FFORMAT
          ENDIF
          CALL PLANTE(1)
          STOP
      END SELECT
!
!-----------------------------------------------------------------------
!
      RETURN
      END
```

Their goal is just to test the format value and redirect to the format-specified implementation of the function.
The modules of the third part contain the implementation of those format specific functions.
Each file is associated to an id which is associated to a Fortran custom-type object defined in the format module. This object contains any information necessary to running Hermes with the format (for example: the number of nodes, elements. . .).

9.3.2 Serafin Format

Format description

The SERAFIN format is a Format Binary file (Each record is written in-between two tags, 4-bytes-integers, containing the size of the record) composed of the list of following records:

- TITLE: title of the mesh (80 characters long)
- NBV1,NBV2: Number of variables: with a linear discretisation, with a quadratic discretisation, NBV2 is now obsolete its value is 0.
- NBV1+NBV2 records:
  - NAME AND UNIT OF A VARIABLE (32 characters long)
- 1,0,0,0,0,0,NPLAN,NPTFR,NPTIR,HAS_DATE: NPLAN is the number of planes this is only in a 3D mesh, NPTFR and NPTIR are only present in a partitioned file they are respectively the number of boundary points and the number of interface points
- If HAS_DATE is not equal to 0 then the following record is in the file:
  YEAR,MONTH,DAY,HOUR,MINUTE,SECOND: date of the creation of the file
- NELEM, NPOIN, NDP, 1: Number of elements, Number of points, number of points per element
- IKLE: connectivity table: array of dimension (NDP,NELEM) whereas in TELEMAC-MASCARET SYSTEM the dimensions are (NELEM,NDP)
- IPOBO/KNOLG: array of integer dimension NPOIN, IPOBO contains 0 for the internal points and it provides a numbering of the boundary points for the others. If the file is partitioned (i.e. parallel run of the code) instead it is called KNOLG and it contains the local to global numbering of the mesh points

- X array of real dimension NPOIN, contains the X coordinates of the mesh points
- Y array of real dimension NPOIN, contains the Y coordinates of the mesh points
- The following are then found for each time step:
  - TIME: a real, time value for the time step
  - Values for variable 1 at time TIME, dimension NPOIN
  - ...
  - Values for variable NBV1+NBV2 at time TIME, dimension NPOIN

New functionalities in Hermes

To allow the Hermes functions to be generic, the way to read/write SERAFIN format was modified. Before Hermes, a normal read/write structure was used, because of that there was a lot of calls to the "rewind" functions and constraints on how to read/write. Especially when reading the data informations as the file was read sequentially (i.e. always starting for the begin of the file and having to skip things to get to the data you wanted).

To change that the "stream" access was used instead, it allows to read the file as a C binary file (i.e. it treats the file as a continuous sequence of bytes, addressable by a positive integer starting from 1). By building a map when opening the file we can have "direct" access to the data needed.

Here below is the object used for the SERAFIN format the first part is the map of the file and the second one some value from the file that are frequently needed so that the file is not reread for those.

A couple of fixed values are also set such as the size of single/double precision for integer and real as well as the size of string (title, variable name and unit...).

```
integer, parameter :: is = 4 ! integer size
integer, parameter :: i4 = selected_int_kind(5) ! integer size
integer, parameter :: i8 = selected_int_kind(15) ! integer on 8 bytes size
integer, parameter :: r4 = selected_real_kind(5) ! single precision size
integer, parameter :: r8 = selected_real_kind(15) ! double precision size
integer, parameter :: var_size = 32 ! size of a variable text
integer, parameter :: title_size = 80 ! size of a title
!
type srf_info
  ! size of elements
  integer :: rs ! real size (4 or 8)
  ! position in file
  integer :: pos_title
  integer :: pos_nvar != pos_title + 4 + title_size + 4
  integer :: pos_varinfo != pos_nvar + 4 + 2*is + 4
  integer :: pos_ib != pos_varinfo + 4 + nvar*var_size + 4
  integer :: pos_date != pos_ib + 4 + 10*is + 4
  integer :: pos_num != pos_date + (ib(10).ne.0)*(4 + 6*is + 4)
  integer :: pos_ikle != pos_num + 4 + 4*is + 4
  integer :: pos_ipobo != pos_ikle + 4 + nelem*ndp*is + 4
  integer :: pos_coord != pos_ipobo + 4 + npoin*is + 4
  integer :: pos_data != pos_coord + (4 + npoin*rs + 4)*ndim
  ! computed informations
  integer :: size_data != 4 + npoin*rs + 4
```

```
  integer :: size_data_set != 4 + rs + 4 + nvar*(4 + npoin*rs + 4)
  ! stocked quantities and small variables
  integer :: ntimestep
  integer :: npoin
  integer :: nvar
  integer :: nelem
  integer :: ndp
  integer :: nplan
  integer :: nptir
  integer :: ndim
  integer :: typ_elt
  character(len=var_size),allocatable :: var_list(:)
  ! boundary informations
  integer :: typ_bnd_elt
  integer :: nptfr
  integer :: ncli
end type srf_info
```

The RS sets the size of the real value (4 for single precision SERAFIN format, 8 for double precision SERAFIND format).

9.3.3 MED format

Format description

The goal of the MED format (EDF and CEA, L-GPL licence) is to standardize exchange of data between scientific computational codes. For instance, this format is used by the SALOME platform (`http://www.salome-platform.org`) to manage transfer between the different modules. The MED format is a compact binary storage of meshes, results and computational data based on the HDF5 library. The generic storage structure of the MED format offers to store several meshes, fields, profiles, groups at different times in the same file. The mesh can be structured or not, based on different elements and can change in time. For HPC aspects, reading and writing can be executed in parallel in the single file. More information can be found in the MED documentation (`http://www.code-aster.org/outils/med/html/index.html`).

New functionalities in Hermes

To adapt to TELEMAC-MASCARET SYSTEM a structure was defined for the boundary file to work with MED. The group structure (which allows to define a list of points/elements as a group) available in MED was used. The MED boundary file follows this structure:

- NGROUP: Number of groups
- LIHBOR,LIUBOR,LIVBOR,LITBOR,GROUP: (Type of boundary on h,u,v,tracer and the name of the group)

Here is a simple example:

```
3
2 2 2 2 BOUNDARY1
5 4 4 4 BOUNDARY2
4 5 5 5 BOUNDARY3
```

9.3.4 How to add a new format

To add a new format (named *format*) the following steps must be fulfilled:

- Create the file "utils_*format*.f" and implement all the functions described in 9.2.1
- Update all the functions generic file to add a new branch to the "if" statement for *format*
- Same thing in `bief\_open\_files.f` and `bief_close_files.f`
- Add in all the dictionary the option to choose *format* for the "FORMAT" keywords

9.3.5 Error Handling

A few error values where created in `declarations_special.f`:

- `HERMES_RECORD_UNKNOWN_ERR`
- `HERMES_VAR_UNKNOWN_ERR`
- `HERMES_FILE_ID_ALREADY_IN_USE_ERR`
- `HERMES_FILE_NOT_OPENED_ERR`
- `HERMES_MAX_FILE_ERR`
- `HERMES_WRONG_ARRAY_SIZE_ERR`
- `HERMES_MED_NOT_LOADED_ERR`
- `HERMES_UNKNOWN_ELEMENT_TYPE_ERR`
- `HERMES_WRONG_ELEMENT_TYPE_ERR`
- `HERMES_UNKNOWN_GROUP_ERR`
- `HERMES_WRONG_HDF_FORMAT_ERR`
- `HERMES_WRONG_MED_FORMAT_ERR`
- `HERMES_WRONG_MED_VERSION_ERR`
- `HERMES_WRONG_AXE_ERR`

9.3.6 Future work

Here is a list of modifications that could be interesting in the future:

- Switch to boundary on elements in Hermes and in TELEMAC-MASCARET SYSTEM
- Add 3D mesh evolving with time (MED only), pending development in ParaVis to handle that
- Use MED possibility to have multiple meshes for coupling

10. CUE

The CUE is the bug/development tracker of TELEMAC-MASCARET SYSTEM. It is available at the following address `cue.opentelemac.org`. In order to login use your SVN login and password.

10.1 Projects

It is divided in multiple projects:

- Modules: Those are the modules in the TELEMAC-MASCARET SYSTEM code.
- Sites: This concern all the development tools (CUE, CIS, Website...).
- Supporting scripts: This concerns all the environment scripts (Python and Perl) as well as parallelism, the automatic installer and the Inputs and Outputs.

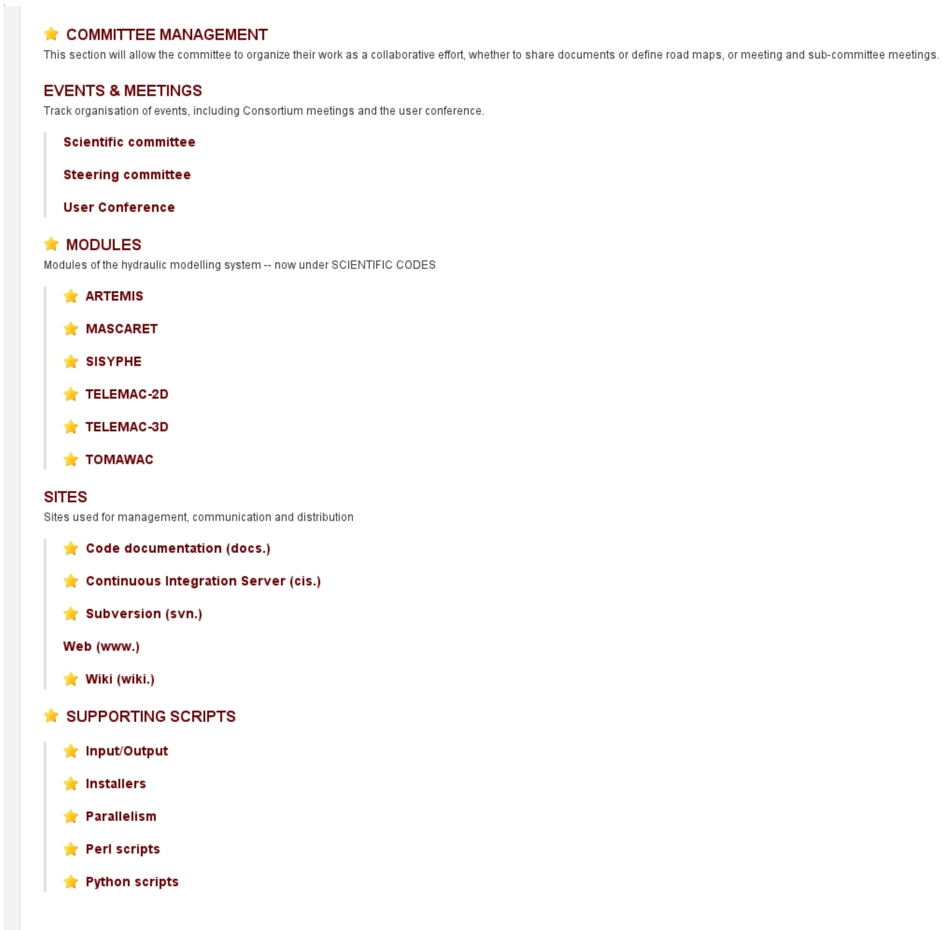

Figure 10.1: CUE projects

10.2 Create a ticket

To add a new ticket you must go into the project your ticket concern and add click on "New issue". This will lead you to the page shown on Fig 10.2. You will then need to fill the following information:

- Tracker: type of the ticket (Bug, Feature, Documentation, Validation/Verif/Application).
- Subject: Title of the ticket.
- Description: Give an full explication of the problem.
- Status: Status of the ticket (Set to new on creation).
- Priority: Urgency of the ticket.
- Assignee: Person in charge of the development integration.
- Category: Category of the work.
- Target Version: Version of the code in which the development should be integrated.
- Watchers: People that will get an update every time the ticket is modified.

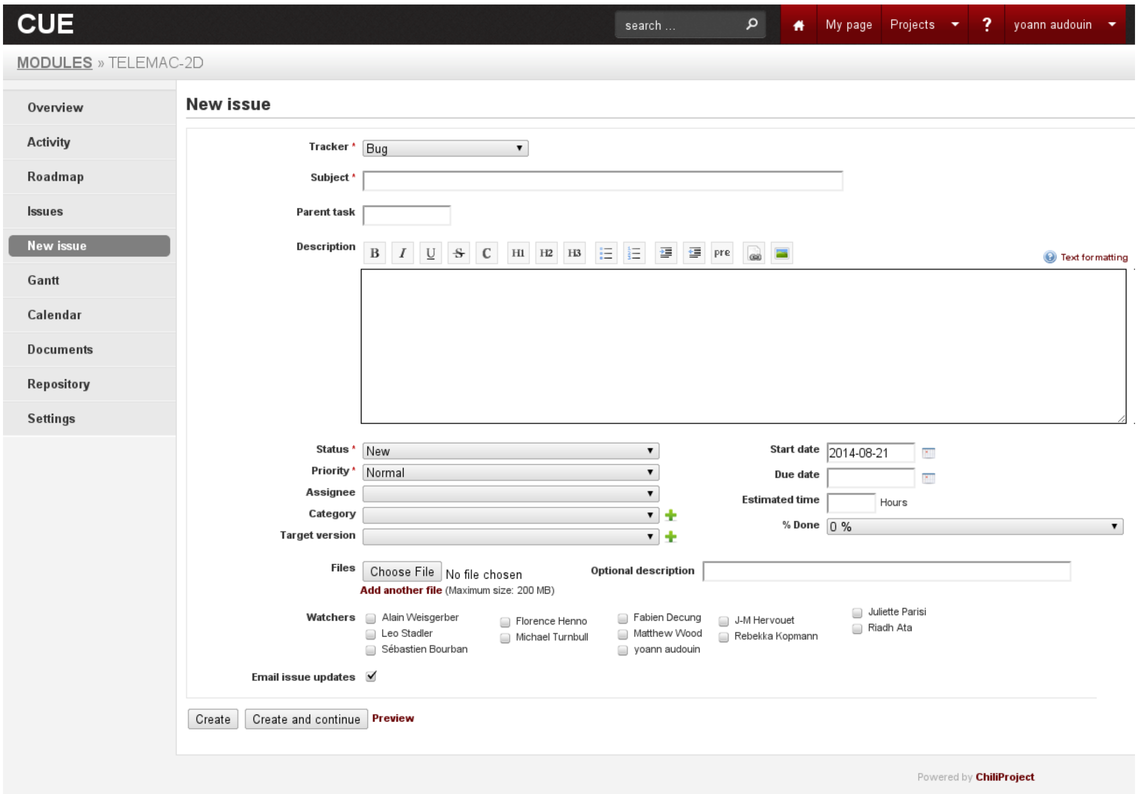

Figure 10.2: Creation of a ticket

Warning:
If you do not see the "New issue" button then you forgot to ask in the email (described in Section 7) the project you are working on, you will need to send a new one to be see that button.

10.3 Modify a ticket

To Modify a ticket go into the project your ticket is in then click on the ticket and on the ticket page click on the "update" button in the upper right corner of the page. The Fig 10.3 shows the page you get when clicking on a ticket.

You will have to update your ticket as your work advance, either by adding comments on what you have done or by changing its status. For example a bug is set to "resolved" once we found its solution and set to "closed" once the correction is integrated in the main version.

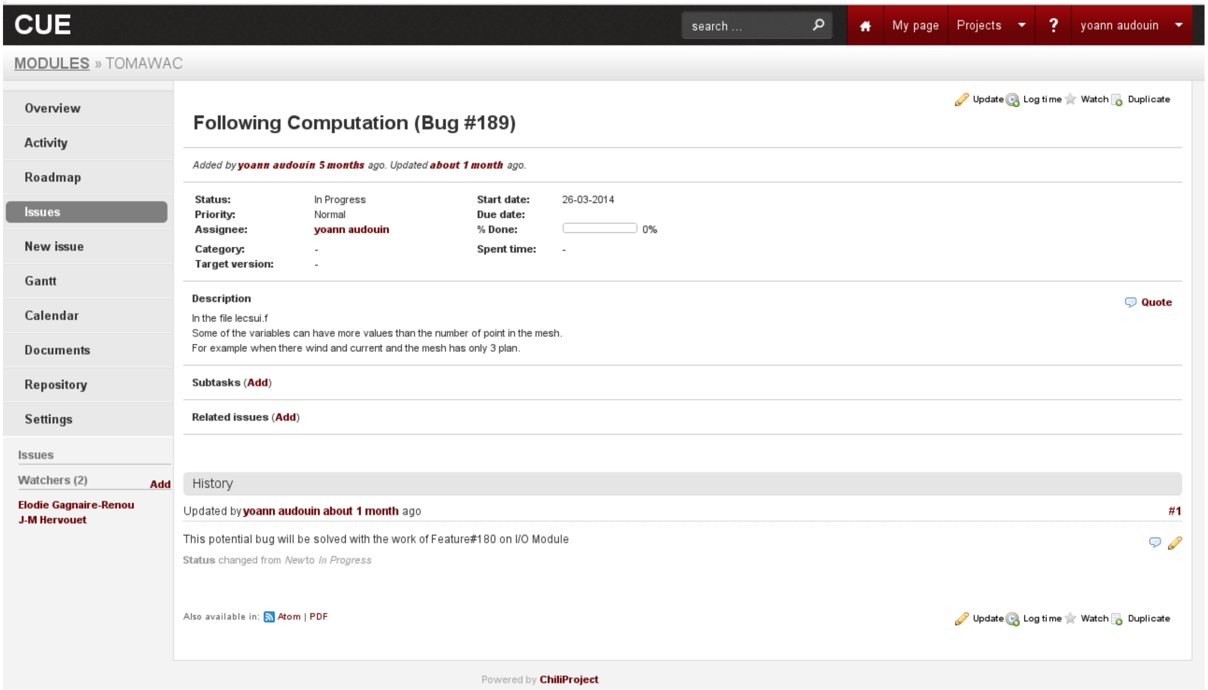

Figure 10.3: Modification of a ticket

11. SVN

SVN is the name of the software we use to control the source of TELEMAC-MASCARET SYSTEM. The link `http://en.wikipedia.org/wiki/Version_control` will give you an explanation of what a source control is. The section below will give you a guide on how to perform a few actions using SVN.

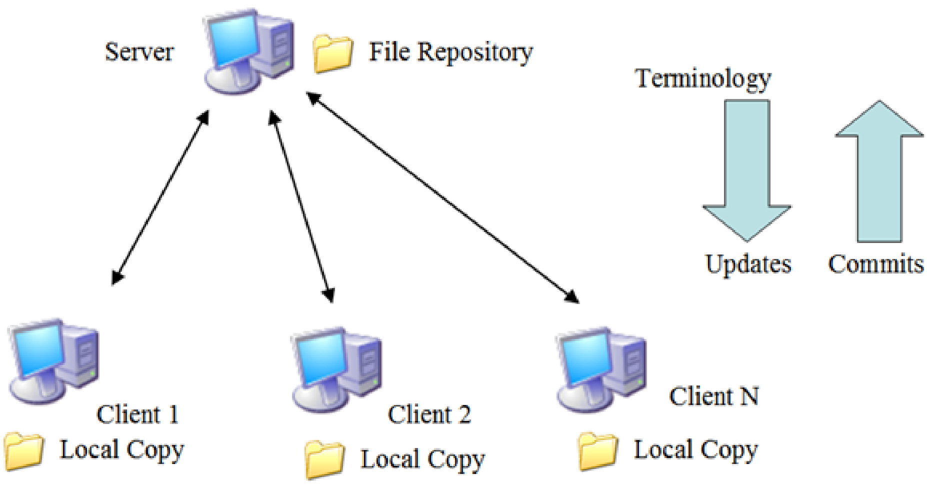

Figure 11.1: SVN structure

If you are not into command line a few software give you a graphical interface to handle your repository: kdeSVN, RapidSVN...

11.1 Create a work copy

```
svn checkout http://svn.opentelemac.org/svn/opentelemac/trunk DEST
```

Create a local repository in *DEST* of the subversion server on the computer. If you want a working copy of your branch just replace `http://svn.opentelemac.org/svn/opentelemac/trunk` by `http://svn.opentelemac.org/svn/opentelemac/branches/branchname` where *branchname* is the name of your branch.

Warning:

If your are using a network proxy you need to modify the `$HOME/.subversion/server` file by adding the following lines under the line `[global]`:

```
[global]
...
http-proxy-host = proxypac.edf.fr
http-proxy-port = 3128
http-proxy-username = NNI
http-proxy-password = SesamePassword
...
```

Where:

- **http-proxy-host** is the address of your proxy.
- **http-proxy-port** is the port of your proxy.
- **http-proxy-username** is the login for your proxy.
- **http-proxy-password** is the password for your proxy.

11.2 SVN commands

Here is a list of a few useful SVN commands:

```
svn help [command]
```

You can get a detailed description of any command.

```
svn update
```

Update your local repository with the server repository. This will add all the modification made on the subversion server on your local repository.

```
svn commit -m "Message about what the commit contains"
```

Push your local modifications on the server repository. This will add all the modifications you made on your local repository on the server repository. You should alway do an update before doing a commit in case someone else did some modifications before you. Anyway if you are not up to date SVN will not allow the commit. The $-m$ option allows you to write directly the message associated with the commit instead of having a text editor opening. Those messages should summarize what the commit is adding.
The message should respect the following template "[*Type*] *Text*" where:

- If you have a cue ticket associated to the commit:
  - Type = "fix #*id*" ,"feature #id" or "vnv #id" where id is the id of the cue ticket
  - Text = Title of the cue ticket
- Otherwise:
  - Type = doc : If ti concerns the documentation
  - Type = scripts : If it concerns the scripts of the system
  - Type = src : General action on the source code (code convention, trimming removing white spaces...)

- Type = vnv : Verification & Validation
- Text = Description of the commit

If the commit contains more than one action repeat the process on a new line.

```
svn log
```

Display all the commit messages.

Tips:

If the output is too big use the following command instead and press q to exit.

```
svn log | less
```

```
svn status
```

Display the status on all the file in the local repository. If a file is modified, added, missing or deleted. See "svn help status" for more information.

```
svn add/delete/move
```

Add/Delete/Move a folder/file to the SVN repository.

```
svn info
```

Display information about the local repository. Like the address of the server repository, the last revision, . . .

```
svn revert FILE
```

Cancel the local modifications on the file *FILE*. This cannot be undone so tread lightly with this command.

11.3 Update your branch with the latest version of the trunk

One of the conditions for validating a development is that it is up to date with the trunk. In order to ease that step that can be some times painful it is recommended to do that action weekly. This way you do smaller updates instead of a massive one.

The commands

1. Go into the branch main folder.

   ```
   cd mybranch
   ```

   Where *mybranch* is the path to your local checkout of your branch.

2. Launch the merge command with *rev* being the last revision of the trunk you are up to date with. If this is the first time you are updating it is the revision at which your branch was created (can be found in the log given by the "svn log" command) otherwise you can get that value using the following command:

   ```
   svn propget svn:mergeinfo .
   ```

   It should return something like that:

```
/branches/guppy:187-256,4145-4591
/branches/jewelpuffer:4665-4793
/branches/rainbowfish:2559-2958,4070-4614,4623-4798
/branches/salmon:138-254,272-286
/trunk:541-3423,4222-4817
```

The value you want is in the line `/trunk:541-3423,4222-4817`. You need the last digits i.e. 4817. Then you replace in the following command rev by that number.

```
svn merge -r rev:HEAD http://svn.opentelemac.org/svn/opentelemac/trunk .
```

The *HEAD* value will be automatically replaced by the latest revision of the trunk.

3. If the merge generates any conflict you will need to resolve them (See Section 11.3).

4. When everything is resolved. You need to commit the merged version. Add the trunk revision number to the commit message for information.

```
svn commit -m "Merged with revision rev of the trunk"
```

Conflicts

When using SVN you sometime encounter a conflict. For example if two persons are working on the same file. You will get the following message:

```
conflict discovered in 'foo.c'.
Select: (p) postpone, (df) diff-full, (e) edit,
        (mc) mine-conflict, (tc) theirs-conflict,
        (s) show all options:
```

Here is a listing of all the options available:

```
(e)  edit             - change merged file in an editor
(df) diff-full        - show all changes made to merged file
(r)  resolved         - accept merged version of file

(dc) display-conflict - show all conflicts (ignoring merged version)
(mc) mine-conflict    - accept my version for all conflicts (same)
(tc) theirs-conflict  - accept their version for all conflicts (same)

(mf) mine-full        - accept my version of entire file (even non-conflicts)
(tf) theirs-full      - accept their version of entire file (same)

(p)  postpone         - mark the conflict to be resolved later
(l)  launch           - launch external tool to resolve conflict
(s)  show all         - show this list
```

If you do not know what to do select option *p*. This option will generate the following files near the one in conflict:

- *foo.c.mine* which contains your local version of the file
- *foo.c.r*44 which contains the file at the last revision on the server repository.
- *foo.c* which contains both of the previous files with the following syntax:

```
<<<<<<< .mine
This is fun stuff!
=======
This is a documentation file
>>>>>>> .r6
```

You need to select in the file what part should be kept. Once the file is correct to resolve the conflict launch the following command:

```
svn resolved foo.c
```

Warning:
"svn resolved" tells SVN that you solved the conflict and that is all. So thread lightly with that option if you call "svn resolved" on a file in which you did not made the modifications it will most likely break the compilation as the "<<<<" will still be in the file.

Tips:
You can add the option "–accept ARG" to the merge command to give an automatic response in case of a conflict.

```
--accept ARG             : Specify the action to apply in case of conflicts
  ('postpone', 'base', 'mine-conflict', 'theirs-conflict',
   'mine-full', 'theirs-full', 'edit', 'launch')
```

11.4 Merge a development into the trunk

The person in charge of the integration will have to follow those steps:

1. Go into the trunk main folder.

   ```
   cd mytrunk
   ```

   Where *mytrunk* is a SVN repository pointing on the trunk. The trunk repository should be clean of every modification to be even more prepared, the command "svn status" should return nothing.

2. Launch the merge command with *rev*1 being the revision at which the development associated with the merge started. The *rev*2 value will be automatically replaced by the latest revision of the branch.

   ```
   svn merge -r rev1:rev2 --reintegrate http://svn.opentelemac.org/svn/opent
   ```

3. If the merge generates any conflict you will need to resolve them (See Section 11.3).

4. The "–reintegrate" option will tell svn to bypass the commit that were merged from the trunk, i.e it will only merge the developments.

5. When everything is okay. You must now commit the merged version. Add the trunk revision number to the commit message for information.

   ```
   svn commit -m "Merged␣of␣branch␣mybranch␣for␣feature␣#???␣of␣the␣cue"
   ```

11.5 Fresh start on branch

You have just finished your development and want to get ready for the next one? To do that efficiently use the following script:

```
#!/bin/bash
if [[ $# -ne 3 ]]; then
  echo 'Usage: freshstart.sh branch-name path-to-branch revision-of-trunk'
  echo 'Usage: freshstart.sh rainbowfish ~/opentelemac/branches/rainbowfish 6
  exit 1
fi
branchname=$1
mybranch=$2
rev=$3
delaysvn=/projets/projets.002/systel.002/bin/delaysvn.sh
# Moving into the branch folder
cd $mybranch
# Removing all local modifications execpt in the "configs" and "builds"folder
svn stat|grep -i ? |grep -vi configs/|grep -vi builds|sed -e "s/^?[ ]*//g"|tr
# Copying all the stuff from the latest revision of the trunk to the branch
~/bin/delaysvn.sh svn export --force http://svn.opentelemac.org/svn/opentelem
# Adding new files
svn stat|grep -i ? |grep -vi configs/|grep -vi builds|sed -e "s/^?[ ]*//g"|tr
# Removing file if necessary
# Running diff between trunk and branch
$delaysvn svn diff http://svn.opentelemac.org/svn/opentelemac/branches/$branch
# Getting the file to delete
grep ^D diff.log |sed -e "s|^D[ ]*http://svn.opentelemac.org/svn/opentelemac/
rm diff.log
# Committting the fresh version
$delaysvn svn commit -m "Fresh start from r$rev"
```

And run the following command:

```
freshstart.sh branch-name path-to-branch revision-of-trunk
```

Where:

- *branch − name* is the name of your branch
- *path − to − branch* is the path on your computer to your branch
- *revision − of − trunk* is the revision of the trunk from which you want a fesh start (This is just used as information for the commit message the revision it is going to use is the latest one)

Warning:
This process will completely erase any modifications you have locally on your repository. The "svn export" command will overwrite your local files with the latest version of the trunk.

Copy the text in a file and run `bash file` with *file* the name of your file. Replace *rev* by the revision of the trunk.

11.6 How to generate the list of your modifications

In this part we will explain how to generate a list of the difference between your branch and the trunk. This list id one of the item necessary to validate your development.

```
svn diff --summarize http://svn.opentelemac.org/svn/opentelemac/trunk http://
```

This command will write the difference into the file "work.diff" and on the standard ouput (i.e. in the terminal).

12. CIS

12.1 Launch a test

To launch a test you must go on the CIS main page then click on your branch tab. This will lead you to the page on Fig 12.1.

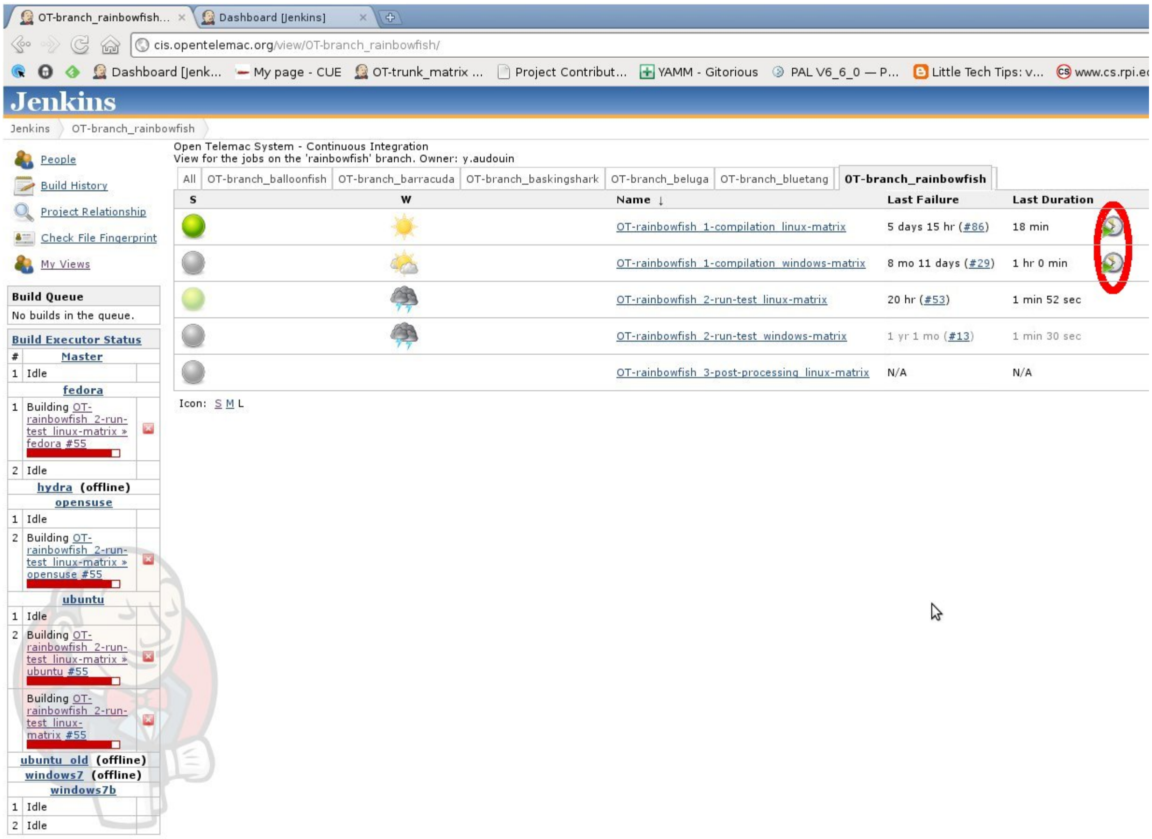

Figure 12.1: CIS Branch Page

Click on the button in the red circle to launch the job. If you do not see that button check that you are logged in. This will lead you to the page on Fig 12.2.

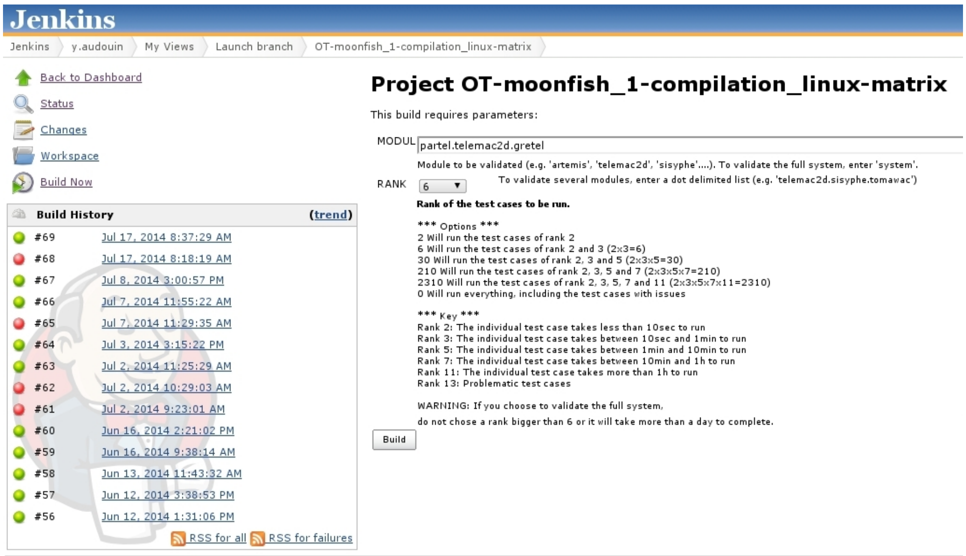

Figure 12.2: CIS Job execution

To run the validation on your branch the following information are needed:

- The modules to run, if you want to run the simulation on only one module do not forget to add partel and gretel as well to be able to run in parallel, for exemple "partel.telemac2d.telemac3d.gretel" will run the validation on telemac2d and telemac3d.

  Writing "system" will run the validation on all the modules this is what you need to validate a development before integration.

- The level of complexity of test cases to run. The higher the number the longer the test cases simulation is. For validation of a development 0 is needed.

If you wanna run the validation locally you need to type one the following commands:

```
validate_telemac.py --tags module
validate_telemac.py --ncsize=3
validate_telemac.py
```

The first one will launch the validate on a specify list of modules (for example "telemac2d", "tomawac artemis"). The second one will launch the validation on the whole system but for the parallel test cases it will replace the number of processors by 3. The third one will run the validation on the whole system

12.2 Get the listing of the test

To see the output of the job you need to follow the step described in Fig 12.3. For step 2 you need to click on the Linux distribution you want want to get the listing from. For information only the ubuntu configuration runs the test cases in parallel.

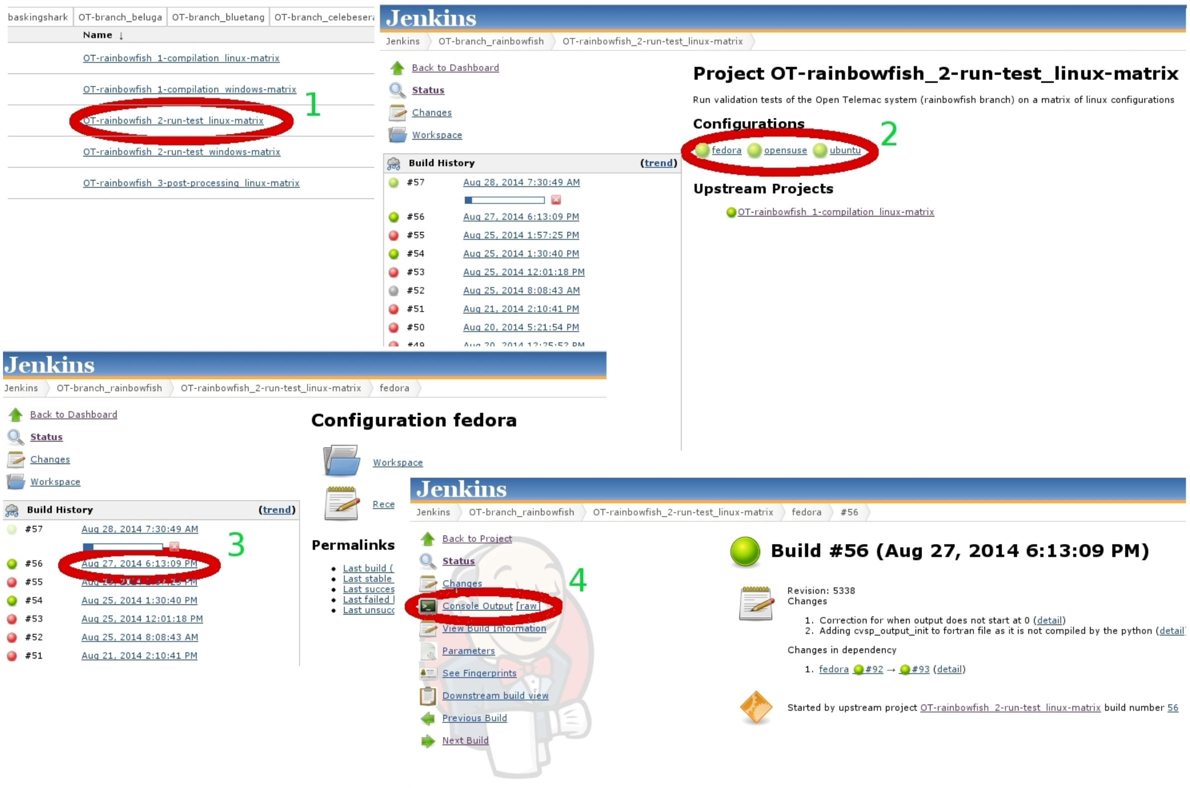

Figure 12.3: Process to get the listing of a job execution

On step 4, clicking on the "raw" button will give you the complete listing as the "Console Output" button will only give you the tail of the output that you can see on Fig 12.4.

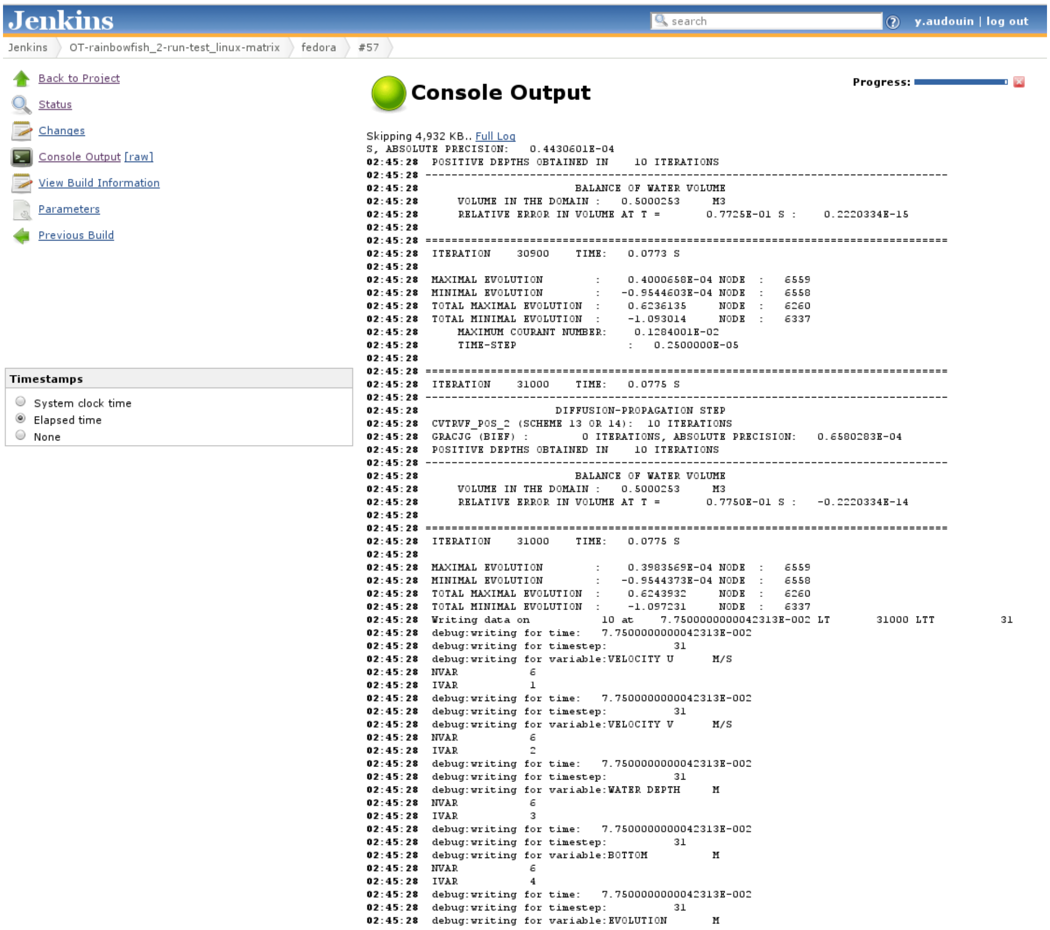

Figure 12.4: Listing of a job execution

13. Code coverage

This chapter will explain how to run the code coverage of the code using gcov and lcov.

13.1 What is Code Coverage

Dixit Wikipedia:"In computer science, code coverage is a measure used to describe the degree to which the source code of a program is tested by a particular test suite. A program with high code coverage, measured as a percentage, has had more of its source code executed during testing which suggests it has a lower chance of containing undetected software bugs compared to a program with low code coverage.Many different metrics can be used to calculate code coverage; some of the most basic are the percent of program subroutines and the percent of program statements called during execution of the test suite."

13.2 What to do

You can find all the information for the configuration in systel.edf.cfg with the configuration gcov.
Then run the following script:

```
#!/bin/bash
# First run to set counter to zero
lcov --directory $HOMETEL/builds/$USETELCFG/lib --capture \
--initial --output-file $HOMETEL/app.info
# Running test cases
validate_telemac.py -k2 --clean --bypass
# Gathering data
lcov --directory $HOMETEL/builds/$USETELCFG/lib --capture \
--output-file $HOMETEL/app.info
# Generating html output
genhtml --legend --highlight \
--output-directory $HOMETEL/documentation/code_coverage \
-t "Telemac-Mascaret V&V code coverage" $HOMETEL/app.info
```

This will build the html display under `<root>/documentation/code_coverage`. That display will contains for each folder of the sources directory the percentage of code/functions used and if you follow through you can even see the file and exactly what line was used.

14. Documentation

This chapter will describe how the documentation is handled in TELEMAC-MASCARET SYSTEM. All the documentation files are written in LaTeXand are using the same Style.

14.1 The structure

All the documentation files can be found in the "documentation" folder at the root of the TELEMAC-MASCARET SYSTEM sources. The first level as a folder for each module plus a Misc Folder which contains all the documentation that are either generic to the while system or not link to a module.
Then for each module we have the following folders:

- reference
- release_note
- user
- validation

Each documentation folder contains those files/folder:

```
main.tex
graphics
-- image.png
latex
-- file.tex
```

Where :

- main.tex The main LaTeXfile.
- graphics Folder contains all the figures associated with the documentation.
- latex Contains all the files that create the documentation.

In **Misc/TelemacTemplateDoc** you can find a template that describes how to write a TELEMAC-MASCARET SYSTEM documentation.

Warning:
The reference documentation is automatically generated from the dictionary of the module so all the modification must be made in the dictionary file.

Warning:
The validation manual merge all the latex contains in the **doc** folder of the test cases.

14.2 How to compile

Everything is done using the python script `doc_telemac.py`. By default it will compile all the documentation. By adding "-m module" it will compile only the documentation for that specific module, by adding "-M miscdoc" it will only compile the documentation "miscdoc" from the **Misc** folder. And the options "–reference,–user…" compile only the reference,user…documentation.

14.3 How to convert a Word documentation into LaTeX using GrindEQ

The main conversion word is made using the software GrindEQ.
Before running the conversion it is strongly suggested to remove the index.
After the conversion is ran all that is left is some search and replace to comply with the template.
Here are a couple of things you will encounter:

- All lot of figure will be created as for a weird reason some letter are represented with pictures. To have the LaTeXfile compile I suggest using a dummy picture and copy it to the according name (it should be image1,image2…).
- Remove all the \
- All the equations should compile directly but you should reorganise them in the LaTeXso they are more readable.

15. Dictionary

This chapter will describe how the dictionary is used in TELEMAC-MASCARET SYSTEM. The dictionary is the input parameter for the reference documentation, the eficas interface and the steering file. The module handling the dictionary is called DAMOCLES and can be found under `sources/utils/damocles`.

15.1 Description of the dictionary

The dictionary is an ASCII file containing a list of keywords for each keyword a number of parameters can be defined. Every line starting with a "/" is considered a comment.

> **Warning**
> No line of the dictionary should be longer that 72 characters.

The first line of a dictionary must always be '&DYN'
Here is a list of those parameters and theirs constraint. Every parameter containing "(opt)" are optional the others are mandatory. The parameters must be added in that order.

NOM It is the name of the keyword in French. It should be max 72 characters long and between "'". If the name contains an apostrophe it should be doubled.

NOM1 It is the name of the keyword in English. It should be max 72 characters long and between "'".

TYPE This is the type of the keyword the TELEMAC-MASCARET SYSTEM handles 4 kind of types:

- **STRING** For text.
- **INTEGER** For integer values.
- **REAL** For real values.
- **LOGICAL** For boolean values.

INDEX This is the index to access that keyword for each type it must be unique. Running DAMOCLES can give you what indexes are available.

TAILLE Number of values expected for the keyword. If the keyword can have a dynamic number of values set TAILLE to 2 and add DYNLIST in APPARENCE.

(opt) SUBMIT This text is only for keywords referring to a file. It is a 6 part chain separated by ";". Here is an example 'T2DBI1-READ;T2DBI1;FACUL;BIN;LIT;SELAFIN'. Each part gives the following information:

- Name of the file in the temporary folder (6 letters long) - opening access (READ for read only, WRITE for write only, READWRITE for both).
- Name of the file in the temporary folder (6 letters long).
- Status of the file (FACUL if the file is optional, OBLIG if it is mandatory).
- Type of the file (BIN for binary, ASC for ASCII file).
- Opening access (LIT for read only, ECR, for write only, ECRLIT for both)
- Special treatment to apply for parallelism:
  - SELAFIN-GEOM: geometry file will go through partel.
  - SELAFIN: mesh file will go through but only the result field will be partitioned it will use the mesh from the SELAFIN-GEOM file.
  - CONLIM: boundary condition file.
  - PARAL: file will be copied for each processor.
  - SCAL: no copy only the main processor will be able to access it.
  - WEIRS, ZONES, SECTIONS: file added to partel with SELAFIN-GEOM.
  - CAS: keyword for the steering file.
  - DICO: keyword for the dictionary.
  - FORTRAN: user fortran.
  - DELWAQHYD, DELWAQSEG ...: files for coupling with Delwaq.

DEFAUT French default value of the keyword. It should contains TAILLE values.

DEFAUT1 English default value of the keyword. It should contains TAILLE values.

MNEMO Name of the variable in the code containing the value of the keyword.

(opt) CONTROLE Two integer that define the min and max of the value of the keyword (This is not used yet).

(opt) CHOIX List of values available for the keyword (in French). If the keyword is a STRING just put the list of values in the following from 'text1';'text2';... You can also use CHOIX to build a association between the actual value and a string by following this syntax: 'val1:"text1"';'val2:"text2"';... You can have a look at the keywords `SOLVER` and `VARIABLES FOR GRAPHIC PRINTOUTS` for examples. Note that the limitation to those choices is not made by DAMOCLES when you are running a case, it is only done by the interface. Text for the value are not allowed to contain apostrophes.

(opt) CHOIX1 Same as CHOIX but in English.

(opt) APPARENCE This is used to give information for the interface on how to enter the values for the keyword the possible values are:

- LIST: To display it in the form of an array.
- TUPLE: To display a couple of values.
- DYNLIST: To display a dynamic list.

RUBRIQUE This is used to categorized the keywords. It should contain three values that are the name of the categories in French.

> **Warning**
> The RUBRIQUE cannot have the same name as a keyword.

RUBRIQUE1 Same RUBRIQUE but in English.

(opt) COMPOSE Not used yet.

(opt) COMPORT Not used yet.

NIVEAU This is the status of the keyword if 0 the keyword will be considered mandatory in the interface. Later it will also be used to group keywords for specific studies.

AIDE Text in French describing what the keyword is used for. This text can use LaTeX format. It will be used to generate the reference documentation.

AIDE1 Same as AIDE but in English.

15.2 Description of the dictionary additional file

This file is only for eficas it is not read during a basic run of TELEMAC-MASCARET SYSTEM. The file is build in two parts:

- The dependencies between keywords (i.e keywords that should appear only if a keyword has a certain value) and "consigne" text that is to be displayed if the keyword as a certain value
- The status of RUBRIQUES.

The first part is a list of blocks for each keyword as they are linked to a keyword. The block for a dependence must follow that syntax:

```
n number_of_the_dependence
condition
keyword_on_which_is_the_condition
keyword_1
keyword_2
...
keyword_n
```

The `number_of_dependence` will be increased as we add blocks for that keyword. The condition must follow a couple rules:

- It must be in Python syntax.
- It must use the "eficas form of the keyword" (i.e. Replace " " "’" "-" by "_").
- If the keyword has a CHOIX it must use the text and not the value.

If the condition is on more than one keyword and affect only one keyword set `number_of_the_dependencie` to 0 and `n` to 1.
The block for a "consigne" must follow that syntax:

```
1 number_of_the_dependence
condition
keyword_on_which_is_the_condition
Text_in_French
Text_in_English
```

The `number_of_dependence` must be negative but still follow the increase (i.e. if its the third dependence it will be -3). Both the text in French and the one in English must be written on one line.
Here is an example for the keyword `INITIAL CONDITIONS` which has 3 dependencies and one "consigne".

```
2 1
INITIAL_CONDITIONS == 'CONSTANT ELEVATION'
INITIAL CONDITIONS
INITIAL ELEVATION
2 2
INITIAL_CONDITIONS == 'CONSTANT DEPTH'
INITIAL CONDITIONS
INITIAL DEPTH
2 3
INITIAL_CONDITIONS == 'TPXO SATELLITE ALTIMETRY'
INITIAL CONDITIONS
ASCII DATABASE FOR TIDE
1 -4
INITIAL_CONDITIONS == 'SPECIAL'
INITIAL CONDITIONS
Les conditions initiales sur la hauteur d''eau doivent etre precisees dans le
The initial conditions with the water depth should be stated in the CONDIN su
```

The second part that is at the end of the file begins with the line:

```
666 666
```

Then it is a list of two lines:

```
NAME_OF_RUBRIQUE
STATUS
```

By default all RUBRIQUE are mandatory here you can change that by setting `STATUS` to `f`. `NAME_OF_RUBRIQUE` must have the same name as in the dictionary.

15.3 What DAMOCLES can do for you

DAMOCLES can be used via the script `damocles.py` and has option for three things:

- –dump, Read a dictionary and dump it back reordered and reorganize.
- –eficas, Generate the Catalogue for eficas to build the interface.
- –latex, Generate a LaTeX file for the reference documentation.

All those options are to be combine with the option `-m` to specify on which module to run the script by default it is run for all of them except MASCARET. The first one can also be used to get information on the dictionary such as the index used, the RUBRIQUE in French and English to check that we have the same number of each the reordered dictionary will be next to the original with a 2 added to the name. It also checks that the dictionary is following the rules described before.
The eficas option is generating all the files needed to run the GUI. All the files are added in the folder eficas in the source folder of the module.
The latex option is used by `doc_telemac.py` to compile the reference manual for that module.

16. Validation

This chapter will describe how to use the validation Python scripts. Those scripts are used to define a VnV (Verification and Validation) test case. It will describe what to run and what to do with the data from the runs such as comparison between reference file and results file, comparison with an analytical solution, comparison with data...

16.1 Structure of Python script

Each test case is described using a Python script that must start with "`vnv_`" and looks like that when empty:

```python
"""
Validation script for gouttedo
"""
from vvytel.vnv_study import AbstractVnvStudy
from execution.telemac_cas import TelemacCas, get_dico
from data_manip.extraction.telemac_file import TelemacFile

class VnvStudy(AbstractVnvStudy):
    """
    Class for validation
    """

    def _init(self):
        """
        Defining general parameters
        """
        self.rank = 4
        self.tags = ['telemac2d']

    def _pre(self):
        """
        Defining the studies
        """
        pass
```

```
    def _check_results(self):
        """
        Check on run results
        """
        pass

    def _post(self):
        """
        Post-treatment processes
        """
        pass
```

This defines a class named "`VnvStudy`" which inherits from "`AbstractVnvStudy`" which is an abstract class for which you need to fill the following 4 functions:

- _init: This is were we define the rank and the tags and optional parameter. Only rank and tags are mandatory.
  - rank: defines the importance of the test case the rule for the rank is described below.
  - tags: While the tag is a system to identify was is tested in the case. This list of tags can be find in `validate_telemac.py`.
  - listing: If set to True will force option -s in execution to write the listing in a file. This is necessary when you are using post-treatment on the listing.
  - walltime: This can be used to force the value of runcode.py potions –walltime. It can be either a str or a dictionary. If it is an str it will apply it to all the studies within the file. If it is a dictionary the keys are a study name and value the associated walltime. This option is only taken into account if you have a cluster configuration.
- _pre: This is were we will defined the studies, a study is defined by a steering file and a module. It can also be given commands which are defined by string that will be executed in the shell.
- _check_results: This is were we will do checks on the results versus, measurements, analytical solutions, reference files...
- _post: This were we will do the post-treatment we recommand to use function from postel Python module but you can use any Python code.

The rank follow the rules below:

- 0: Minimal validation should last less than an hour and check each module.
- 1: More complete validation should last less than 4 hours.
- 2: Less than a day (Daily validation).
- 3: The additional test launch over the WE.
- 4: Very specific cases run only we are making a new release.

16.2 Where to look for examples

You can have a look at all the Python script in the examples but here is a small list of where to find examples on how to do specific actions:

- For a basic validation case (steering file run in sequential and parallel and comparison of sequential vs reference, parallel vs reference and sequential vs parallle) as well as a couple examples of post-treatment have a look at `examples/telemac2d/gouttedo/vnv_thompson.py`
- For an example of a validation against an analytical solutions and the post-treatment to go with that have a look at `examples/telemac2d/thacker/vnv_thacker.py`
- For an example of the generation of multiple steering file to test a range of options have a look at `examples/telemac3d/lock-exchange/vnv_lock_exchange_sensibility.py`

For examples of extractions and post-treatment have a look at the notebooks (In notebooks at the root of your TELEMAC-MASCARET SYSTEM). To run them use jupyter notebook and run `jupyter notebook notebooks/index.ipynb`.

16.3 How to run validation

To run validation use the script "`validate_telemac.py`". To summarise what you have access to:

- if you pass the script Python file as argument it will run them otherwise it will loop over the ones in the examples folder.
- if you add -k/–rank or –tags you can specify for which ranks, tags to run validation.
- if you add –vnv-pre/–vnv-run/–vnv-post/–vnv-check-results you can run only those steps (you can have more than). Just beware that some are necessary for the others (for example you can not do post treatment if you have not run the case first). The pre-treatment phase is always run.
- if you add –report-name=toto it will generate a csv file at the root of your TELEMAC-MASCARET SYSTEM containing time informations for each step (pre, check_results) and the run of each study.
- if you add –clean or –full-clean instead of running it will delete the files created by the validation script (this will delete the results of the runs).
- all the options from `runcode.py`. Those will be passed to each run.

When running "`validate_telemac.py`" on an already ran VnV case the run part will not be done if none of the input files (files to read given in the steering file) or the steering file itself are newer than one the output files (a file that was generated by the run).
To see all the options run `validate_telemac.py -h`.

16.3.1 Validation on cluster

Validation can also run on cluster for more efficiency. It will follow this pattern:

1. Clean up the examples folder
2. Launch all the TELEMAC-MASCARET runs via the scheduler
3. Wait for the jobs to be finished
4. Launch the epsilons check and the post-treatment

Requirements

To run validation on a cluster first you'll have to have a configuration with the following points:

- A hpc configuration (see on the website for more information).
- The batch submission command must write in a file for each submission the id of the submission and the folder of case ';' separated.

The procedure below will submit each of the TELEMAC-MASCARET studies to the cluster scheduler. This means that in the best of case your whole validation will be as long as your longest TELEMAC-MASCARET run. The "commands" with the argument hpc=True will be submetted as well.
Here is an example for a cluster using slurm (The command is a one line command it is on multiple line here):

```
cp HPC_STDIN ../;
cd ../;
ret=‘sbatch --wckey="P119C:TELEMAC_SYSTEM" < HPC_STDIN‘;
id=‘echo $ret|tr ' ' '\n'|tail -n 1‘;
dir=‘readlink -f .‘;
echo "$id;$dir" >> <id_log>;
echo $ret
```

`<id_log>` will be replace by the options in `validate_telemac.py` if given otherwise it we be replace by 'id.log'.
Here is an extract of what the file containing the id looks like (the paths have been shortened to find in the documentation):

```
30346528;.../trunk/examples/artemis/G8M/vnv_g8m/vnv_1/eole.intel.dyn
30346529;.../trunk/examples/artemis/beach/vnv_beach/vnv_1/eole.intel.dyn
30346531;.../trunk/examples/artemis/beach/vnv_beach/vnv_2/eole.intel.dyn
30346534;.../trunk/examples/artemis/bj78/vnv_bj78/vnv_1/eole.intel.dyn
30346535;.../trunk/examples/artemis/bj78/vnv_bj78/vnv_2/eole.intel.dyn
30346537;.../trunk/examples/artemis/bosse/vnv_bosse/vnv_1/eole.intel.dyn
38368703;cmd:.../trunk/examples/artemis/bj78/vnv_bj78.py:vnv_1_api
38368704;cmd:.../trunk/examples/artemis/bj78/vnv_bj78.py:vnv_2_api
```

Run commands

The procedure to run is the following:

1. Run '`validate\_telemac.py` *valid_options* `--clean`'.
2. Run '`validate\_telemac.py` *valid_options* *hpc_options* `--vnv-mode=slurm`'.

Replacing:

- *valid_options* by the options for your validation (–tag, -k, –bypass...).
- *hpc_options* by the options you would give a hpc TELEMAC-MASCARET run on your cluster (–queue, –nctile, –walltime, –jobname...).

17. Usefull stuff

17.1 Little script to check part of the coding convention

In the trunk version or after (V7.0) you can find a script called `check_code.sh` that will scan your source code and check for a few points of the coding convention. You should run this script before submitting your development. Below is the description the script will give you if you launch it with the `-h` option. This script is located under the `scripts` folder in the TELEMAC-MASCARET SYSTEM directory.

```
Script checking some points of the coding convention
for all the ".f" and ".F" in the folder given in parameter
It will generate those files:
-- cc_0-invalid-char.log: checks that there are no tabs
                          or CLRF (Windows \n)
-- cc_1-indent.log: contains the line where the
                    indentation is not a 6 + x*2
-- cc_2-comment.log: checks that the character used
                     for comments is '!'
-- cc_3-continuation.log: checks that the character
                          for continuation is '&'
-- cc_4-lower-case.log: checks that there are
                        no lowercase code
-- cc_5-line-too-long.log: checks that there are no
                           line wider than 72
                           character (expect comments)
-- cc_6-encoding.log: checks that there are no files
                      which encoding does not
                      support utf8
```

17.2 Adding a new test case

This section will guide you through the hard but needed action of adding a new case do not frighten it is not that hard. First of all you need to create a new folder in the examples in the folder corresponding to the module the test case is for. That folder must contain the following elements:

- All the **input** files you need to run the case, and just the input the files generated by a successful run should not be in the SVN repository. See the table 17.1 below for the convention for the naming of the files.
- A reference file and/or data to do the validation.
- The `doc` folder which contains the documentation for the test case in LaTeX format (See other test cases for example).
- The xml file to run the test case (See other test cases for example).

All the Serafin file must have the extension "slf", the steering case the extension "cas".

Table 17.1: Table with contents ranging over several cells horizontally and vertically.

	geometry, boundary	reference	results	restart	steering and others
TELEMAC-2D	geo	f2d	r2d	i2d	t2d
TELEMAC-3D	geo	f3d	r3d	i3d	t3d
TOMAWAC	geo	f2d	r2d	ini	tom
STBTEL	geo	ref	r2d	ini	stb
GAIA	geo	gai_ref	gai	ini	gai
SISYPHE	geo	fis	rsi	ini	sis
POSTEL-3D	geo	ref	res	xxx	p3d
WAQTEL	geo	ref	raq	ini	waq
ARTEMIS	geo	frt	r2d	ini	art

18. Matrix storage conventions

The off-diagonal terms of a matrix A are placed in a two-dimensional array, the first dimension being NELMAX, the maximum number of elements (the second dimension depends on the type of matrix and storage). The following conventions are written in the form of rows, such that:

```
XA(IELEM,01)  = XA12
```

This row means the following:
The contribution of element IELEM to the coefficient of point 2 in the equation for point 1 is placed in XA(IELEM,01). 1 and 2 refer to the local numbering of element IELEM, and so the general number of point 1 is IKLE(IELEM,1).
The location is also given in the form of a matrix whose elements give the second dimension of XA in which the corresponding term is placed. These matrices are indeed used in BIEF, in which they are given in the form of DATA tables. In view of FORTRAN placing notation for two-dimensional arrays, the matrices appear in transposed form. For this reason, the transposed form of the matrices is also given here.

18.1 Triangle P1-P1 EBE

$$\begin{pmatrix} - & 1 & 2 \\ 4 & - & 3 \\ 5 & 6 & - \end{pmatrix} \text{transposed form: } \begin{pmatrix} - & 4 & 5 \\ 1 & - & 6 \\ 2 & 3 & - \end{pmatrix}$$

```
XA(IELEM,1)  = XA12
XA(IELEM,2)  = XA13
XA(IELEM,3)  = XA23
```

If A is asymmetrical:

```
XA(IELEM,04)  = XA21
XA(IELEM,05)  = XA31
XA(IELEM,06)  = XA32
```

18.2 Triangle P1-Quasi-bubble EBE

$$\begin{pmatrix} - & 1 & 2 & 3 \\ 4 & - & 5 & 6 \\ 7 & 8 & - & 9 \end{pmatrix} \text{transposed form: } \begin{pmatrix} - & 4 & 7 \\ 1 & - & 8 \\ 2 & 5 & - \\ 3 & 6 & 9 \end{pmatrix}$$

```
XA(IELEM,01) = XA12
XA(IELEM,02) = XA13
XA(IELEM,03) = XA14
XA(IELEM,04) = XA21
XA(IELEM,05) = XA23
XA(IELEM,06) = XA24
XA(IELEM,07) = XA31
XA(IELEM,08) = XA32
XA(IELEM,09) = XA34
```

18.3 Triangle Quasi-bubble-P1 EBE

$$\begin{pmatrix} - & 1 & 2 \\ 3 & - & 4 \\ 5 & 6 & - \\ 7 & 8 & 9 \end{pmatrix} \text{transposed form: } \begin{pmatrix} - & 3 & 5 & 7 \\ 1 & - & 6 & 8 \\ 2 & 4 & - & 9 \end{pmatrix}$$

```
XA(IELEM,01) = XA12
XA(IELEM,02) = XA13
XA(IELEM,03) = XA21
XA(IELEM,04) = XA23
XA(IELEM,05) = XA31
XA(IELEM,06) = XA32
XA(IELEM,07) = XA41
XA(IELEM,08) = XA42
XA(IELEM,09) = XA43
```

18.4 Triangle Quasi-bubble Quasi-bubble or Quadrilateral Q1-Q1 EBE

$$\begin{pmatrix} - & 1 & 2 & 3 \\ 7 & - & 4 & 5 \\ 8 & 10 & - & 6 \\ 9 & 11 & 12 & - \end{pmatrix} \text{transposed form : } \begin{pmatrix} - & 7 & 8 & 9 \\ 1 & - & 10 & 11 \\ 2 & 4 & - & 12 \\ 3 & 5 & 6 & - \end{pmatrix}$$

```
XA(IELEM,01) = XA12
XA(IELEM,02) = XA13
XA(IELEM,03) = XA14
XA(IELEM,04) = XA23
XA(IELEM,05) = XA24
XA(IELEM,06) = XA34
```

If A is asymmetrical:

```
XA(IELEM,07) = XA21
XA(IELEM,08) = XA31
XA(IELEM,09) = XA41
XA(IELEM,10) = XA32
XA(IELEM,11) = XA42
XA(IELEM,12) = XA43
```

18.5 Triangle P1 EBE - Quadratic triangle EBE

$$\begin{pmatrix} - & 1 & 2 & 3 & 4 & 5 \\ 6 & - & 7 & 8 & 9 & 10 \\ 11 & 12 & - & 13 & 14 & 15 \end{pmatrix}$$

```
XA(IELEM,01) = XA12
XA(IELEM,02) = XA13
XA(IELEM,03) = XA14
XA(IELEM,04) = XA15
XA(IELEM,05) = XA16
XA(IELEM,06) = XA21
XA(IELEM,07) = XA23
XA(IELEM,08) = XA24
XA(IELEM,09) = XA25
XA(IELEM,10) = XA26
XA(IELEM,11) = XA31
XA(IELEM,12) = XA32
XA(IELEM,13) = XA34
XA(IELEM,14) = XA35
XA(IELEM,15) = XA36
```

18.6 Quadratic triangle EBE - Triangle P1 EBE

$$\begin{pmatrix} - & 1 & 2 \\ 3 & - & 4 \\ 5 & 6 & - \\ 7 & 8 & 9 \\ 10 & 11 & 12 \\ 13 & 14 & 15 \end{pmatrix}$$

```
XA(IELEM,01) = XA12
XA(IELEM,02) = XA13
XA(IELEM,03) = XA21
XA(IELEM,04) = XA23
XA(IELEM,05) = XA31
XA(IELEM,06) = XA32
XA(IELEM,07) = XA41
XA(IELEM,08) = XA42
XA(IELEM,09) = XA43
XA(IELEM,10) = XA51
XA(IELEM,11) = XA52
XA(IELEM,12) = XA53
XA(IELEM,13) = XA61
XA(IELEM,14) = XA62
XA(IELEM,15) = XA63
```

18.7 Prism P1-P1 EBE or Quadratic triangle EBE

$$\begin{pmatrix} - & 1 & 2 & 3 & 4 & 5 \\ 16 & - & 6 & 7 & 8 & 9 \\ 17 & 21 & - & 10 & 11 & 12 \\ 18 & 22 & 25 & - & 13 & 14 \\ 19 & 23 & 26 & 28 & - & 15 \\ 20 & 24 & 27 & 29 & 30 & - \end{pmatrix}$$

transposed form:

$$\begin{pmatrix} - & 16 & 17 & 18 & 19 & 20 \\ 1 & - & 21 & 22 & 23 & 24 \\ 2 & 6 & - & 25 & 26 & 27 \\ 3 & 7 & 10 & - & 28 & 29 \\ 4 & 8 & 11 & 13 & - & 30 \\ 5 & 9 & 12 & 14 & 15 & - \end{pmatrix}$$

```
XA(IELEM,01) = XA12
XA(IELEM,02) = XA13
XA(IELEM,03) = XA14
XA(IELEM,04) = XA15
XA(IELEM,05) = XA16
XA(IELEM,06) = XA23
XA(IELEM,07) = XA24
XA(IELEM,08) = XA25
XA(IELEM,09) = XA26
XA(IELEM,10) = XA34
XA(IELEM,11) = XA35
XA(IELEM,12) = XA36
XA(IELEM,13) = XA45
XA(IELEM,14) = XA46
XA(IELEM,15) = XA56
```

If A is asymmetrical:

```
XA(IELEM,16) = XA21
XA(IELEM,17) = XA31
XA(IELEM,18) = XA41
XA(IELEM,19) = XA51
XA(IELEM,20) = XA61
XA(IELEM,21) = XA32
XA(IELEM,22) = XA42
XA(IELEM,23) = XA52
XA(IELEM,24) = XA62
XA(IELEM,25) = XA43
XA(IELEM,26) = XA53
XA(IELEM,27) = XA63
XA(IELEM,28) = XA54
XA(IELEM,29) = XA64
XA(IELEM,30) = XA65
```

19. The SELAFIN format

Note: for unclear historical reasons this format is also sometimes called SERAFIN
This is a binary file.
This format can be 'SERAFIN ', for single precision storage, or 'SERAFIND' for double precision storage. Double precision storage can be used for cleaner restarts, but may not be understood by all post-processors.
All string in the SERAFIN file must be utf-8 encoded (See for `https://en.wikipedia.org/wiki/UTF-8` for the exact list).
The records are listed below. Records are given in the FORTRAN sense. It means that every record corresponds to a FORTRAN WRITE:
1 record containing the title of the study (80 characters), The last 8 characters must contain the format of the file (SERAFIN or SERAFIND)
1 record containing the two integers NBV(1) and NBV(2) (NBV(1) the number of variables, NBV(2) with the value of 0),
NBV(1) records containing the names and units of each variable (over 32 characters),
1 record containing the integers table IPARAM (10 integers, of which only 4 are currently being used).
If IPARAM (3) is not 0: the value corresponds to the x-coordinate of the origin in the mesh
If IPARAM (4) is not 0: the value corresponds to the y-coordinate of the origin in the mesh
These coordinates in metres may be used by post-processors to retrieve geo-referenced coordinates, while the coordinates of the mesh are relative to keep more digits.
If IPARAM (7) is not 0: the value corresponds to the number of planes on the vertical (in prisms.)
If IPARAM (8) is not 0: the value corresponds to the number of boundary points (in parallel).
If IPARAM (9) is not 0: the value corresponds to the number of interface points (in parallel).
if IPARAM (10) = 1: a record containing the computation starting date in 6 integers: year, month, day, hour, minute, second
1 record containing the integers NELEM,NPOIN,NDP,1 (number of elements, number of points, number of points per element and the value 1),
1 record containing table IKLE (integer array of dimension (NDP,NELEM) which is the connectivity table. Beware: in TELEMAC-2D, the dimensions of this array are (NELEM,NDP)),
1 record containing table IPOBO (integer array of dimension NPOIN); the value is 0 for an internal point, and gives the numbering of boundary points for the others. This array is never used (its data can be retrieved by another way). In parallel the table KNOLG is given instead, keeping track of the global numbers of points in the original mesh.

1 record containing table X (real array of dimension NPOIN containing the abscissas of the points),
1 record containing table Y (real array of dimension NPOIN containing the ordinates of the points),
Next, for each time step, the following are found:

- 1 record containing time T (real),
- NBV(1)+NBV(2) records containing the results arrays for each variable at time T.

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