Operator `CALCULATION`

1 Goal

For mechanics:

- C alculer internal constraints and variables for the integration of a non-linear law of behavior;
- C alculer elementary vectors `vect_elem` internal and nodal forces and elementary matrices `matr_elem` of a tangent matrix;
- C alcule R elementary vectors `vect_elem` forces corresponding to the variables of order.

For thermics:

- to calculate the elementary vectors `vect_elem` residues of balance and matrices elementary `matr_elem` of a thermal matrix of rigidity;
- C alcule R elementary vectors `vect_elem` forces corresponding with the non-linear thermal loadings.

Product a structure of data of the type `table_container`.

2 Syntax

```
table_container        = CALCULATION
   (  ♦ MODEL          = Mo,                          [model]
      ♦ CHAM_MATER     = chmat,                       [cham_mater]
      ◊ CARA_ELEM      = carac,                       [cara_elem]
      ◊ TABLE          = table,                       [table_container]
      ♦ INCREMENT      = _F (
              ♦ LIST_INST = litps,                    [listr8]
              ♦ NUME_ORDRE =nuini,                    [I]
            ),
      ◊ PHENOMENON     =/'MECHANICAL'                 [DEFECT]
                        /'THERMAL'

    If PHENOMENON = 'MECHANICAL'
      {
       ♦ OPTION        =   /'BEHAVIOR'             [DEFECT]
                           /'MATR_TANG_ELEM'
                           /'FORC_INTE_ELEM'
                           /'FORC_NODA_ELEM'
                           /'FORC_VARC_ELEM_M'
                           /'FORC_VARC_ELEM_P'
      ◊ EXCIT          = _F (
              ♦ LOAD  = chi,                       [char_meca]
              ◊ FONC_MULT =fi,                        [fonction/formule]
            ),
      ♦ BEHAVIOR   =_F (see the document [U4.51.11]),
      ◊ SCHEMA_THM     =_F (see the document [U4.51.11]),
      ◊ DEPL           = depl,                        [cham_no]
      ◊ INCR_DEPL      = incdepl,                     [cham_no]
      ◊ SIGM           = sigm,                        [cham_elem]
      ◊ VARI           = vari,                        [cham_elem]
       ◊ MODE_FOURIER   = nh ,                           [I]
       }
    If PHENOMENON = ' THERMICS '
      {
       ♦ OPTION        =   /' CHAR_THER_ELEM '
                           /'MATR_TANG_ELEM'
                           /'CHAR_EVOL_ELEM'
                           /'RESI_THER_ELEM'
      ♦ EXCIT          = _F (
              ♦ LOAD  = chi,                       [char_ther]
              ◊ FONC_MULT =fi,                        [fonction/formule]
            ),
      ♦ TEMP           = temp,                        [cham_no]
      ♦ INCR_TEMP      = Inctemp,                     [cham_no]
      ♦ BEHAVIOR   =_F (see the document [U4.54.02]),
      ◊ PARM_THETA     =/ theta,                      [R]
                        /0.57,                        [DEFECT]
       }


      ◊ INFORMATION    =   /1,                                  [DEFECT]
                  /2,
   )
```

3 Operands commun runs

3.1 Keyword PHENOMENON

```
◊ PHENOMENON    =/ 'MECHANICAL'                    [DEFECT]
                  /'THERMAL'
```

Allows to choose the phenomenon which will be calculated.

3.2 Keyword TABLE

♦ `TABLE`

Allows to introduce one `table_container` not-vacuum to supplement (with the adequate sequence number) with the new concepts calculated in the operand `CALCULATION`.
If the table contains already fields for the sequence number claimed by the keyword `INCREMENT/NUMÉRIQUE_ORDRE` , these fields are crushed and an alarm is emitted to warn the user.

3.3 Keyword MODEL

♦ `MODEL = Mo`

Name of the concept defining the model whose elements are the object of calculation.

3.4 Keyword CHAM_MATER

♦ `CHAM_MATER = chmat`

Name of the concept defining the affected material field on the model `Mo`.

3.5 Keyword CARA_ELEM

◊ `CARA_ELEM = carac`

Name of the concept defining the characteristics of the elements of beam, hulls, etc…

3.6 Keyword INCREMENT

♦ `INCREMENT`

Defines the time intervals taken in the incremental method.

In mechanics, Lurgent be thus defined have physical direction only for relations of behavior where time intervenes explicitly (viscoelastic or viscoplastic for example). In the other cases, they allow only indicer the increments of load and to parameterize the evolution of a possible field of temperature.

3.6.1 Operand LIST_INST

♦ `LIST_INST = litps`

The moments of calculation are those defined in the concept `litps` by the operator `DEFI_LIST_REEL` [U4.34.01].

3.6.2 Operands NUME_ORDRE

♦ `NUME_ORDRE = digital`

Allows to define the sequence number (and thus the moment) for which will be calculated the sizes in `table_container`.

3.7 Operand INFORMATION

◊ `INFORMATION = inf`

Allows to carry out in the file message various intermediate impressions.

4 Operands for mechanics

4.1 Keyword EXCIT

◊ EXCIT

This keyword factor makes it possible to describe with each occurrence a load (requests and boundary conditions), and possibly a multiplying coefficient and/or a kind of load.
This keyword is useful to produce the matrix of the dualized limiting conditions of Dirichlet which will be integrated in matr_elem product by the calculation of the tangent matrix.

4.1.1 Operand LOAD

♦ LOAD: CH $_I$

CH_I is the mechanical loading (possibly comprising the evolution of a field of temperature) specified with i ème occurrence of EXCIT.

4.1.2 Operand FONC_MULT

◊ FONC_MULT: F $_I$

F_I is the multiplying function of the time of the loading specified with Ième occurrence of EXCIT.
The loading and boundary conditions for n occurrences of the keyword factor EXCIT are:

$$ch=\sum_{i=1}^{n} f_i . ch_i$$

For the conditions of Dirichlet, of course, only the specified value is multiplied by F_I.
By default: F_I=1.

4.2 Operand OPTION

```
♦ OPTION    =  /'BEHAVIOR'   [defect]
               /'MATR_TANG_ELEM'
               /'FORC_INTE_ELEM'
               /'FORC_NODA_ELEM'
               /'FORC_VARC_ELEM_M'
               /'FORC_VARC_ELEM_P'
```

Allows to specify what one calculates:

- 'BEHAVIOR' integrate the law of behavior and thus produces three objects: cham_elem constraints, cham_elem internal variables and one cham_elem comprising the code return of the law of behavior;
- 'MATR_TANG_ELEM' calculate the coherent tangent matrix (option FULL_MECA) and thus produces four objects: one cham_elem constraints, one cham_elem internal variables, one cham_elem comprising the code return of the law of behavior and one matr_elem tangent elementary matrices;
- 'FORC_INTE_ELEM' calculate the vector of the internal forces after integration of the law of behavior (RAPH_MECA in the language Aster) and thus produces four objects: one cham_elem constraints, one cham_elem internal variables, one cham_elem comprising the code return of the law of behavior and one vect_elem elementary vectors of the internal forces;
- 'FORC_NODA_ELEM' calculate the vector of the nodal forces starting from the constraints at the points of Gauss and produces one vect_elem elementary vectors of the nodal forces.
- 'FORC_VARC_ELEM_M' calculate the vector of the forces corresponding to the variables of orders at previous time (given by LIST_INST). See the related paragraph in the theoretical documentation of STAT_NON_LINE [R5.03.01].
- 'FORC_VARC_ELEM_P' calculate the vector of the forces corresponding to the variables of orders at time running (given by LIST_INST). See the related paragraph in the theoretical documentation of STAT_NON_LINE [R5.03.01].

4.3 Keyword DEPL/INCR_DEPL/SIGM/VARI

```
◊ DEPL       = depl,      [cham_no],
◊ INCR_DEPL  = incdepl,   [cham_no],
◊ SIGM       = sigm,      [cham_elem],
◊ VARI       = vari,      [cham_elem],
```

Allows to introduce inlet limits to calculate the various fields by the order CALCULATION :

- DEPL give a field of displacement;
- INCR_DEPL is the increment of the field of displacement since the beginning of the step of time;
- SIGM give a stress field;
- VARI give a field of internal variables.

Note:

It is necessary to take care to be coherent between the behavior requested by BEHAVIOR and field of the internal variables cuts it.
*The field of the constraints being used to calculate the option FORC_NODA_ELEM is not the same one according to calculations requested. Indeed, if one integrates the law of behavior (options BEHAVIOR, MATR_TANG_ELEM, FORC_INTE_ELEM), then the stress field taken in the calculation of the option FORC_NODA_ELEM will be that calculated **afterwards** the integration of the behavior. In this case, SIGM is the tensor of the constraints **initial** and will not be that employed in the calculation of FORC_NODA_ELEM. On the other hand, if only the option FORC_NODA_ELEM is asked, then one will use the field of the constraints directly given by SIGM.*

4.4 Operand MODE_FOURIER

◊ MODE_FOURIER = nh

Positive or null entirety indicating the harmonic of FOURIER on whom one calculates the elementary vector for an axisymmetric model 2D.

5 Operands for thermics

5.1 Keyword `EXCIT`

◊ `EXCIT`

This keyword factor makes it possible to describe with each occurrence a load (requests and boundary conditions), and possibly a multiplying coefficient and/or a kind of load.
This keyword is useful to produce the matrix of the dualized limiting conditions of Dirichlet which will be integrated in `matr_elem` product by the calculation of the matrix of thermal rigidity.

5.1.1 Operand `LOAD`

♦ `LOAD: CH` $_I$

Concept of the type `load` product by `AFFE_CHAR_THER` or by `AFFE_CHAR_THER_F` [U4.44.02].

Notice important:

> *For each occurrence of the keyword factor `EXCIT` various concepts `tank` used must be built on the same model `Mo` .*

5.1.2 Operand `FONC_MULT`

◊ `FONC_MULT: F` $_I$

Multiplicative coefficient function of time (concept of the type `function, tablecloth or formula`) applied to the load.

Notice important:

> *The concomitant use of `FONC_MULT` with a load containing of the thermal loadings depending on the temperature is prohibited; i.e. for loadings of the type `ECHANGE_` , `RADIATION, SOUR_NL` or `FLUNL` .*

5.2 Operand `OPTION`

```
♦ OPTION    =  /'CHAR_THER_ELEM'
               /'MATR_TANG_ELEM'
               /'CHAR_EVOL_ELEM'
               /'TANK_RESI_ELEM'
```

Allows to specify what one calculates:

- `'CHAR_THER_ELEM'` calculate them `vect_elem` corresponding to the non-linear thermal loadings (`SOURCE_NL`, `RADIATION` and `FLUX_NL`). For the linear loadings, it will be necessary to use `CALC_VECT_ELEM` ;
- `'MATR_TANG_ELEM'` calculate the matrix DE thermal rigidity non-linear and thus produces `matr_elem` elementary matrices. These matrices comprises the voluminal terms of the variational form but also the terms coming from the contribution of the loadings[1] : `EXCHANGE`, `ECHANGE_PAROI`, `RADIATION`, `FLUX_NL` and `SOUR_NL`. If the loadings understand conditions of the Dirichlet type (`AFFE_CHAR_THER/DDL_IMPO`), one has also matrices of dualisation coming from the multipliers of Lagrange;
- `'TANK_EVOL_ELEM'` calculate Lbe `vect_elem` elementary vectors corresponding to the resolution of the transitory problem in time ;
- `'TANK_RESI_ELEM'` calculate Lbe `vect_elem` elementary vectors corresponding to the deficit of balance of the residues for the non-linear coefficients of the thermal parameters (conductivity thermics for example).

1 For `FLUX_NL` and `SOUR_NL` only if the coefficients are functions

5.3 Keyword TEMP/INCR_TEMP

```
◊ TEMP       = temp,      [cham_no],
◊ INCR_TEMP  = Inctemp,   [cham_no],
```

Allows to introduce inlet limits to calculate the various fields by the order CALCULATION :

- TEMP give a field of temperature;
- INCR_TEMP is the increment of the field of temperature since the beginning of the step of time;

5.4 Operand PARM_THETA

```
◊ PARM_THETA = theta
```

The argument theta is the parameter of the theta-method applied to the evolutionary problem. It must be ranging between 0 (explicit method) and 1 (completely implicit method). In the absence, keyword, the value used is $\theta=0.57$, a little higher than $\theta=0.5$ corresponds to the diagram of Crank-Nicholson. The incidence of the choice of theta on the stability of the method is detailed in [R5.02.02].

6 Use of CALCULATION and of table_container

CALCULATION only a table_container produces in which is stored for each sequence number one or more fields (forced, internal variables, elementary vectors of the internal forces, elementary matrices of the tangent matrix).

To extract these fields, it is advisable to use the order EXTR_TABLE. For example, if one wants the field of the constraints resulting from the order CALCULATION, one will make:

```
CONT=CALCUL (OPTION= ('BEHAVIOR', 'FORC_INTE_ELEM', 'MATR_TANG_ELEM'),
             MODELE=MO,
             CHAM_MATER=CHMAT,
             INCREMENT=_F (LIST_INST=LISTE,
                           NUME_ORDRE=1),
             EXCIT=_F (CHARGE=CHARGE),
             DEPL=U,
             INCR_DEPL=DU,
             SIGM=SIGP,
             VARI=VARIP,
             COMPORTEMENT=_F (RELATION=' VMIS_ISOT_LINE',),
             INFO=2,);

SIGM=EXTR_TABLE (TYPE_RESU=' CHAM_GD_SDASTER',
                 TABLE=CONT,
                 NOM_PARA=' NOM_SD',
                 FILTRE=_F (NOM_PARA=' NOM_OBJET',
                            VALE_K=' SIEF_ELGA'),)
```

To calculate the second member of the external forces or other quantities (like the matrices masses), one can use the orders CALC_VECT_ELEM or CALC_MATR_ELEM.
matr_elem or them vect_elem can be assembled via the orders ASSE_VECTEUR and ASSE_MATRICE.

It should be noted that them MATR_ELEM of rigidity produced by CALCULATION contain also the contribution resulting from the dualisation of the limiting conditions of Dirichlet (EXCIT).

An example of use of CALCULATION for mechanics ESt available in the CAS-test pynl01a.