

Operator CALC_ERREUR

1 Goal

To create or supplement one `result` by calculating fields by element of error of discretization.

Note: CALC_ERREUR cannot be used on several processors.

Contents

1 Goal.....	1
2 Syntax.....	3
2.1 Operands RESULTAT/MODELE/CHAM_MATER/CARA_ELEM/EXCIT/SOLVEUR.....	5
2.1.1 Operands RESULT.....	5
2.1.2 Operands MODEL/CHAM_MATER/CARA_ELEM.....	5
2.1.3 Keyword EXCIT.....	5
2.1.4 Keyword SOLVEUR.....	5
2.2 Selection of the sequence numbers.....	5
2.3 Operands for the mechanical options.....	6
2.3.1 Options of calculation of indicators of error.....	6
2.4 Operands for the thermal options.....	9
2.4.1 Operand OPTION.....	9
2.5 Operand TITLE.....	9

2 Syntax

```

resu  [*] = CALC_ERREUR

(
  ◇ reuse = resu,
  ◇ MODEL = Mo, [model]
  ◇ CHAM_MATER = chmater, [cham_mater]
  ◇ CARA_ELEM = carac, [cara_elem]
  ◇ SOLVEUR = _F (see the document [U4.50.01]),
  ◇ EXCIT = _F (
    ◆ LOAD = l_charge, [l_char_meca]
    ◇ / COEF_MULT = cm, [R]
      / COEF_MULT_C= cmc, [C]
      / FONC_MULT = Fm, [function]
      / FONC_MULT_C= FMC, [fonction_C]
    ◇ PHAS_DEG = Pd, [R]
    ◇ PUIS_PULS = N, [I]
    ◇ TYPE_CHARGE = 'FIXES',
  )
  ◇ # Selection of the meshes concerned with calculation
    / ALL = 'YES', [DEFECT]

  ◆ # Selection of the sequence number:
    / TOUT_ORDRE = 'YES',
    / NUME_ORDRE = l_nuor, [l_I]
    / LIST_ORDRE = l_nuor, [listis]
    / NUME_MODE = l_numo, [l_I]
    / NOEUD_CMP = l_nomo, [l_K16]
    / NOM_CAS = nocas, [K16]
    / ◆ / INST = l_inst, [l_R]
      / FREQ = l_freq, [l_R]
      / LIST_INST = l_inst, [listr8]
      / LIST_FREQ = l_freq, [listr8]
    ◇ | PRECISION = / prec,
      / 1.0E-3, [DEFECT]
      | CRITERION = / 'RELATIVE', [DEFECT]
      / 'ABSOLUTE',

# mechanical options
  ◆ RESULT = resu,
    ◆ OPTION = | 'SIZ1_NOEU'
              | 'ERZ1_ELEM'
              | 'SIZ2_NOEU'
              | 'ERZ2_ELEM'
              | 'ERME_ELEM'
              | 'ERME_ELNO'
              | 'ERME_NOEU'
              | 'QIZ1_ELEM'
              | 'QIZ2_ELEM'
              | 'QIRE_ELEM'
              | 'QIRE_ELNO'
              | 'QIRE_NOEU'
              | 'SING_ELEM'
    ◆ PREC_ERR = err [R]
    ◇ TYPE_ESTI = / 'ERME_ELEM',
                  / 'ERZ1_ELEM',
                  / 'ERZ2_ELEM',
                  / 'QIRE_ELEM',
                  / 'QIZ1_ELEM',

```

```

/ 'QIZ2_ELEM' ,

# thermal options
  ◆ RESULT = resu, / [evol_ther]
  ◆ OPTION = | 'ERTH_ELEM' ,
              | 'ERTH_ELNO' ,
              | 'ERTH_NOEU' ,

  ◇ TITLE = title , [l_Kn]
  ◇ INFORMATION = / 1,

[DEFECT]
/ 2,

);
```

2.1 Operands

RESULTAT/MODELE/CHAM_MATER/CARA_ELEM/EXCIT/SOLVEUR

2.1.1 Operands RESULT

◆ RESULT = resu

Name of the structure of data result to enrich. This argument can be same as that used for the concept enriched by the operator, or a different name, which will create a new structure of data result (see for example test SSLS504 [V3.03.504]).

Notice :

In the majority of the situations, the structure of data `resu` contains all the necessary information with the calculation of the options: the model, the field of material, characteristics elementary, loadings. Keywords `MODEL`, `CHAM_MATER`, `CARA_ELEM` and `EXCIT` are thus useless.

2.1.2 Operands MODEL/CHAM_MATER/CARA_ELEM.

◇ MODEL = Mo

Name of the model on which the efforts are calculated, the constraints, deformations,.... It is optional because can be extracted the result.

◇ CHAM_MATER = chmater

Material field associated with the model `Mo`. This keyword is optional, and must be provided only in exceptional cases (voluntary modification of material for example).

◇ CARA_ELEM = carac

Elementary characteristics associated with the model `Mo`, if it contains elements of structure or if the isoparametric elements are affected by a local reference mark of anisotropy. This keyword is optional.

2.1.3 Keyword EXCIT

This keyword factor (optional) makes it possible to specify the thermal or mechanical loadings to use for the calculation of the options, instead of those which were useful in the structural analysis of data specified under the keyword `RESULT`.

The definition of this keyword is identical to that of the orders which built the structure of data `resu` : to see the orders `MECA_STATIQUE` [U4.51.01], `STAT_NON_LINE` [U4.51.03], `DYNA_LINE_HARM` [U4.53.11], and `DYNA_LINE_TRAN` [U4.53.02].

2.1.4 Keyword SOLVEUR

The syntax of this keyword common to several orders is described in the document [U4.50.01].

Note:

In the order, the solver is used only for the estimator of error 'ZZ1'. The authorized solveurs are 'GCPC', 'LDLT', 'MULT_FRONT' (defect), 'MUMPS' and 'PETSC'.

2.2 Selection of the sequence numbers

Use of the keywords `TOUT_ORDRE`, `NUM_ORDRE`, `INST`, `FREQ` is described in the document [U4.71.00].

2.3 Operands for the mechanical options

2.3.1 Options of calculation of indicators of error

| 'ERZ1_ELEM' (respectively 'ERZ2_ELEM')

Calculation of the estimator of error of ZHU-ZIENKIEWICZ (linear elasticity 2D and 3D for version 1, linear elasticity 2D for version 2) starting from the option 'SIZ1_NOEU' (respectively 'SIZ2_NOEU'). If this last field does not exist in `resu`, it is automatically built as a preliminary, to see [R4.10.01].

| 'ERME_ELEM'

Estimator of error in residue in mechanics [R4.10.02] and hydro-mechanical stationary [R4.10.04] calculated by element.

The Councils of use of the option ERME_ELEM

For carrying out well the estimate of error of mechanical calculation (within the theoretical limits of the formula developed within the elliptic framework with regular border....), it should be carried out on all the model:

ALL = 'YES' (value by default)

It should be noted that the model is not inevitably defined on all the geometry.

One also needs the calculation of the constraints to the nodes (confer [R3.06.03]), by SIGM_ELNO. If this stress field to the nodes already does not exist in the structure of data `result`, it is automatically calculated in CALC_ERREUR.

- With regard to the loadings:

It is necessary to provide to CALC_ERREUR loadings used for mechanical calculation:

EXCIT=_F (CHARGE=...)

while taking well keeps with the rules of overloads different for the mechanical solver and this option from CALC_ERREUR.

Thus, mechanical calculation (MECA_STATIQUE, STAT_NON_LINE ...) incorporate the boundary conditions whereas the error analysis will not retain, for a kind of boundary conditions given, that the last listed in EXCIT of CALC_ERREUR. The order thus has a crucial importance! One thus should, for a kind of boundary conditions, only one occurrence in AFFE_CHAR ...

One takes account only loadings of the type: GRAVITY, ROTATION, FORCE_INTERNE, PRES_REP, FORCE_FACE, FORCE_ARETE.

Only the three last can be variable.

It is advised to use finite elements of order two in the case of voluminal forces, if not this term is very badly calculated since the divergence of the tensor of the constraint $\text{div}(\sigma)$ is quasi worthless!

To take into account the error relative to a worthless boundary condition, it should be forced as a function via one AFFE_CHAR_MECA_F. Via a constant, she will not be taken into account.

- Grid:

The grid must be triangular, quadrangle, tetrahedral or hexahedral, with any GROUP_NO if one wants to re-mesh then via LOBSTER.

- In 2D, he takes into account only the errors on (and between) isoparametric elements SEG2/3, TRIA3/6, QUAD4/8/9.

In 3D, idem with FACE3/6/4/8/9, TETRA4/10, PENTA6/13/15, HEXA8/20/27 and PYRAM5/13 but not the elements of structure (hull, plate, beam...).

- In addition, it is necessary to take care not to intercalate segments between two quadrangles or two triangles (respectively QUAD or triangle between two HEXA), if not one cannot calculate the term of jump relative to this vicinity. In the place, one inquires (wrongly) of a possible boundary condition.

| `ERME_ELNO`

Estimator of error in residue calculated with the nodes by element [R4.10.02].

| `ERME_NOEU`

Estimator of error in residue calculated with the nodes.

| `QIZ1_ELEM` (respectively `QIZ2_ELEM`)

Estimator of error in quantities of interest based on the method of Zhu-Zienkiewicz (linear elasticity 2D).

| `QIRE_ELEM`

Estimator of error in quantities of interest based on the residues in mechanics, calculated by element.

The Council of use of the options `QIZ1_ELEM`, `QIZ2_ELEM`, `QIRE_ELEM`

The field of application of the options `QIZ1_ELEM` and `QIZ2_ELEM` is the same one as for the options `ERZ1_ELEM` and `ERZ2_ELEM` and that of L' option `QIRE_ELEM` as that of L' option is the same one `ERME_ELEM` in mechanics.

It is necessary to define, besides the initial problem (primal problem), a second problem (dual problem). This problem defines in a subjacent way the quantity of interest on which one wants to obtain an error. To date, only two quantities of interest are available:

- Average of a component of displacement;
- Average of a component of the tensor of the constraints.

The dual problem differs from the primal problem **only** by its loading (this one being quantity of interest), **conditions of edges remaining the same ones**. Thus the loading to be imposed on the wanted under-field, by the means of the order `AFPE_CHAR_MECA`, is:

- `FORCE_INTERNE`, unit effort for the desired component of displacement;
- `PRE_EPSI`, unit strain for the desired component of the tensor of the constraints.

Once the two solved problems, one calculates for each of both the estimator of "classical" error desired (the same one for both...) and finally new should be defined `CALC_ERREUR` with one of the options of calculation of estimator of error in quantity of interest.

An example of use of the calculation of the estimator in quantities of interest based on the residues can be found in the test `sslv113c` and `sslv113d`.

| `QIRE_ELNO`

Estimator of error in quantities of interest based on the residues calculated with the nodes by element.

| `QIRE_NOEU`

Estimator of error in quantities of interest based on the residues calculated with the nodes.

| `SIZ1_NOEU`

Calculation of the constraints to the nodes (linear elasticity 2D and 3D); the constraints are obtained by a total smoothing (within the meaning of least squares) of the constraints at the points of `GAUSS`. See Estimate of error by smoothing of the constraints [R4.10.01].

| `SIZ2_NOEU`

Calculation of the constraints to the nodes (linear elasticity 2D); the constraints are obtained by a local smoothing with a patch of elements (within the meaning of least squares) of the constraints at the points of GAUSS, to see [R4.10.01].

```
| `SING_ELEM'  
  ◆ PREC_ERR = err [R]  
  ◇ TYPE_ESTI = `ERME_ELEM',  
                `ERZ1_ELEM',  
                `ERZ2_ELEM',  
                `QIRE_ELEM',  
                `QIZ1_ELEM',  
                `QIZ2_ELEM',
```

This option ([R4.10.04]) aims at improving the treatment of the singularities in the strategies of adaptation of grid (in fact with LOBSTER). In practice the indicators of error are high in the singular zones so that quickly only the singular zones are refined and mask thus the other sensitive areas (zones with strong gradient) which one would wish to refine.

This option is a constant field by element and comprises three components:

- 1) `DEGREE' who corresponds to the detection of the singular finite elements. In practice, this component is worth the degree of interpolation of the selected finite elements if the finite element is connected to no singularity and is worth the order of the singularity if the finite element is connected to a node considered by the method as singular (for example for an element close to the point of a crack, this value is worth 0.5).
- 2) `REPORT' who corresponds to the map of modification of size of the finite elements in the event of mending of meshes for a given total error. This component is equal to the relationship between the new size of the finite element and the current size.
- 3) `SIZE' who corresponds to the map of the new sizes of the finite elements in the event of mending of meshes for a given total error. This data is directly usable by certain mailleurs (GMSH for example)

This option can be used according to two diagrams:

- The finite elements considered as "singular" by the method can be excluded from the process of cutting (in their affecting for example a worthless error),
- the new size of the finite elements is given to a remaillor (in fact LOBSTER for Code_Aster) so that this one builds the new grid by as well as possible respecting this new map of size. Currently, the software LOBSTER cuts out the element once (for example into 2D, a triangle is divided into 4 but not more). To continue cutting, it is necessary to call on LOBSTER again. An evolution is thus to envisage so that one can divide several times an element and thus as well as possible respect the map of size of the new grid.

The calculation of this option requires, as a preliminary, the calculation of an indicator of error (it is the absolute component which is used and it is coded in the source of Aster) and of the total deformation energy. If one of these options is not calculated, a message of alarm is transmitted and the option `SING_ELEM' is not calculated.

- For the indicator of error, four choices are possible:
 - `ERME_ELEM' for the indicator in residues,
 - `ERZ (1 or 2) _ELEM_SIGM' for the indicator of Zhu-Zienkiewicz (versions 1 or 2),
 - `QIRE_ELEM' for the indicator in quantity of interest based on the residues,
 - `QIZ (1 or 2) _ELEM_SIGM' for the indicator in quantity of interest based on Zhu-Zienkiewicz (versions 1 or 2),
 - If the six indicators are present and that nothing is specified with `TYPE_ESTI', the indicator in residue `ERME_ELEM' by default (message of emitted alarm) is selected. If the two indicators of Zhu-Zienkiewicz are present, one chooses `ERZ1_ELEM'.
- For the total deformation energy, one uses:

- With `STAT_NON_LINE` : `'ETOT_ELEM'` who is the total deformation energy on a finite element (valid for an elastic behavior and an elastoplastic behavior `'VMIS_ISOT_XXX'`).
- With `MECA_STATIQUE` : `'EPOT_ELEM'` who is the potential energy of elastic strain on a finite element and integrated starting from displacements and temperature (valid only for one elastic behavior).

The user must also inform the keyword `'PREC_ERR'` (a fatal message is transmitted in the event of absence) which makes it possible to calculate the precision desired on the total error to determine the map of modification of size (cf [R4.10.04]). The value of `'PREC_ERR'` strictly lies between 0 and 1 (a fatal message is transmitted if this condition is not checked).

The perimeter of use is the same one (but more reduced) than that of the indicator of error chosen namely:

- For the indicator in residue: finite elements of the continuous mediums in 2D (triangles and quadrangles) or 3D (only tetrahedrons) for an elastoplastic behavior,
- For the indicator of Zhu-Zienkiewicz: finite elements of the continuous mediums in 2D (triangles and quadrangles) for an elastic behavior.

In any rigour, calculation about the singularity is obtained starting from theoretical energy at a peak of crack, valid equation only in elasticity. The use of this option in elastoplasticity is thus to handle with prudence.

| `'SING_ELNO'`

Detection of the singularities and map of modification of sizes to the nodes by element. The preliminary calculation of `'SING_ELEM'` is thus necessary. If `'SING_ELEM'` is absent, a message of alarm is transmitted and the option `'SING_ELNO'` is not calculated.

2.4 Operands for the thermal options

2.4.1 Operand `OPTION`

| `'ERTH_ELEM'`
| `'ERTH_ELNO'`
| `'ERTH_NOEU'`

Estimators of error in residue in thermics calculated starting from flows with the nodes [R4.10.03]. If the calculation of flows to the nodes is not carried out beforehand in the order `CALC_CHAMP` via `FLUX_ELNO`, it is automatically carried out in `CALC_ERREUR`.

The keyword `INFORMATION` get all intermediate postings of calculations (connectivities, normals, diameters, values of the fields, jacobien).

The option `'ERTH_ELNO'` allows to bring back the field by element `ERTH_ELEM` a field with the nodes by element has, which makes it possible to make statements of values or impressions / visualizations.

The option `'ERTH_NOEU'` allows to transform the field with the nodes by element into a field with the nodes.

2.5 Operand `TITLE`

◇ `TITLE = title`

Title which one wants to give to the result of the order [U4.02.01].