

Operator CALC_ERREUR

1 Drank

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

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2 Syntax

```

resu      [*] = CALC_ERREUR

          (
            ◊reuse = resu,
            ◊MODELE =mo , [model]
            ◊CHAM_MATER =chmater , [cham_mater]
            ◊CARA_ELEM =carac ,
[cara_elem]
            ◊SOLVEUR = _F (see the document [U4.50.01]),
            ◊EXCIT = _F (
              ◊CHARGE = l_charge, [l_char_meca]
                ◊/ COEF_MULT = cm, [R]
                  /COEF_MULT_C= cmc, [C]
                  /FONC_MULT = Fm, [function]
                  /FONC_MULT_C= FMC, [function_C]
                ◊PHAS_DEG = Pd, [R]
                ◊PUIS_PULS = N , [I]
                ◊TYPE_CHARGE = "FIXES",
              )
            ◊#Sélection of meshes concerned with /TOUT
              computation = ' OUI',
[DEFAULT]

            ◊#Sélection of sequence number:
              /TOUT_ORDRE = ' OUI',
              /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]
              ◊ | P RECISION = prec,
                /1.0E-3, [DEFAULT]
              | CRITERE = "RELATIF", [DEFAULT]
                /"ABSOLU",
          )

# options mechanical
  ◊RESULTAT =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",

#options thermal
  ◆RESULTAT=resu , /
[evol_ther]
  ◆OPTION= | ' EARTH_ELEM',
           | " EARTH_ELNO",
           | " EARTH_NOEU",

  ◇TITER= titrate , [1_Kn]
  ◇INFO=/1 ,

[DEFAULT]

/2 ,

);
```

2.1 Operands

RESULTAT/MODELE/CHAM_MATER/CARA_ELEM/EXCIT/solver

2.1.1 Operands RESULTAT

◆RESULTAT =resu

Name of data structure result to enriching. This argument can be same as that used for the concept enriched by the operator, or a different name, which will create a new data structure result (see for example test SLS504 [V3.03.504]).

Note:

In the majority of the situations, the data structure `resu` contains all the necessary information with the computation of the options: the model, the material field, characteristics elementary, loadings. The key words `MODELS`, `CHAM_MATER`, `CARA_ELEM` and `EXCIT` are thus useless.

2.1.2 Operands MODELS/CHAM_MATER/CARA_ELEM.

◇MODELE = Mo

Name of the model on which the forces are calculated, the stresses, strains,... It is optional because can be extracted result.

◇CHAM_MATER = chmater

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

Characteristic ◇CARA_ELEM =

carac elementary associated with the model `Mo`, if it contains structural elements or if the isoparametric elements are affected by a local coordinate system of anisotropy. This key word is optional.

2.1.3 Key word EXCIT

This key word factor (optional) makes it possible to specify the thermal or mechanical loadings to use for the computation of the options, instead of those which were useful in computation of data structure specified under key word `RESULTAT`.

The definition of this key word is identical to that of the commands which built the data structure `resu`: to see commands `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 Key word solver

the syntax of this key word common to several commands is described in the document [U4.50.01].

Note:

In the command, the solver is used only for the estimator of error "ZZ1". The authorized solvers are "PCG", "LDLT", "MULT_FRONT" (default), "MUMPS" and "PETSC".

2.2 Selection of the sequence numbers

the use of key words `TOUT_ORDRE`, `NUM_ORDRE`, `INST`, `FREQ` is described in the document [U4.71.00].

2.3 Operands for the mechanical options

2.3.1 Computation options of error indicators

| ' ERZ1_ELEM' (respectively "ERZ2_ELEM")

Computation of the estimator of error of ZHU-ZIENKIEWICZ (elasticity linear 2D and 3D for version 1, linear elasticity 2D for the version 2) from 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 steady [R4.10.04] calculated by element.

The Councils of use of option ERME_ELEM

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

TOUT = "OUI" (default value)

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

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

- With regard to the loadings:
It is necessary to provide to `CALC_ERREUR` the loadings used for mechanical computation:
`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 computation (`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 the `EXCIT` of `CALC_ERREUR`. The order thus has a crucial importance! Is not thus needed, for a kind of boundary conditions, that only one occurrence in the `AFFE_CHAR` ...

One takes account only loadings of the type: `PESANTEUR`, `ROTATION`, `FORCE_INTERNE`, `PRES_REP`, `FORCE_FACE`, `FORCE_ARETE`.
Only the three last can be variable.

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

To take into account the error relative to a boundary condition null, it should be imposed as a function via an `AFFE_CHAR_MECA_F`. Via a constant, she will not be taken into account.

- Mesh:
The mesh must be triangular, quadrangle, tetrahedral or hexahedral, with any `GROUP_NO` if one wants to re-mesh then via `HOMARD`.
- 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 structural elements (shell, 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. With core, 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 options "QIZ1_ELEM", "QIZ2_ELEM", "QIRE_ELEM"

the field of application of options "QIZ1_ELEM" and "QIZ2_ELEM" is the same one as for options "ERZ1_ELEM" and "ERZ2_ELEM" and that of option "QIRE_ELEM" are the same one as that of option "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 stresses.

The dual problem differs from the primal problem **only** by its loading (this one being quantity of interest), **the edge conditions remaining the same ones**. Thus the loading to be imposed on the wanted subdomain, by the means of the command AFFE_CHAR_MECA, is:

- FORCE_INTERNE, unit force for the desired component of displacement;
- PRE_EPSI, unit strain for the desired component of the tensor of the stresses.

Once the two solved problems, one calculates for each of both the estimator of "classical" error desired (the same one for both...) and finally it is necessary to define a new CALC_ERREUR with one of the computation options of estimator of error in quantity of interest.

An example of use of the computation 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 '

Computation of the nodal stresses (linear elasticity 2D and 3D); the stresses are obtained by a total lissage (within the meaning of the least squares) of the stresses to Gauss points. See Estimate of error by lissage of the stresses [R4.10.01].

| ' SIZ2_NOEU '

Computation of the nodal stresses (linear elasticity 2D); the stresses are obtained by a local lissage with a patch of elements (within the meaning of the least squares) of the stresses to Gauss points, 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 processing of the singularities in the strategies of mesh adaptation (in the occurrence with HOMARD). In practice the error indicators 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) "DEGRE" which corresponds to detection of the finite elements singular. In practice, this component is worth the degree of interpolation of the finite elements selected 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) "RATIO" which corresponds to the card 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) "TAILLE" which corresponds to the card 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 mesh generators (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 an error null),
- the new size of the finite elements is given to a remaillor (in fact HOMARD for Code_Aster) so that this one builds the new mesh by as well as possible respecting this new card of size. Currently, the software HOMARD 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 HOMARD again. An evolution is thus to envisage so that one can divide several times an element and thus as well as possible respect the card of size of the new mesh.

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

- For the error indicator, 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" is chosen by default (transmitted alarm message). If the two indicators of Zhu-Zienkiewicz are present, one chooses "ERZ1_ELEM".
- For total strain energy, one uses:

- With STAT_NON_LINE: "ETOT_ELEM" which is total strain energy on a finite element (valid for an elastic behavior and an elastoplastic behavior "VMIS_ISOT_XXX").
- With MECA_STATIQUE: "EPOT_ELEM" which 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 key word "PREC_ERR" (a fatal message is transmitted in the event of absence) which makes it possible to calculate the accuracy desired on the total error to determine the card 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 error indicator chosen namely:

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

In any rigor, computation about the singularity is obtained 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 card of modification of sizes to the nodes by element. The computation preliminary of "SING_ELEM" is thus necessary. If "SING_ELEM" is absent, an alarm message is transmitted and option "SING_ELNO" is not calculated.

2.4 Operands for the thermal options

2.4.1 Operand OPTION

| ' EARTH_ELEM '
| ' EARTH_ELNO '
| ' EARTH_NOEU '

Estimators of error in residue in thermal calculated starting from flux with the nodes [R4.10.03]. If the computation of flux to the nodes is not carried out beforehand in command CALC_CHAMP via FLUX_ELNO, it is automatically carried out in CALC_ERREUR.

Key word INFO gets all the intermediate displays of computations (connectivities, norms, diameters, values of the fields, jacobian).

Option "EARTH_ELNO" makes it possible to bring back the field by element EARTH_ELEM has a field at nodes by element, which makes it possible to make statements of values or printings /visualizations.

Option "EARTH_NOEU" makes it possible to transform the field at nodes by element into a field at nodes.

2.5 Operand TITER

◇TITER = title

Titrate that one wants to give to result of the command [U4.02.01].