Code_Aster

Titre : Conseils d'utilisation de STAT_NON_LINE
Responsable : GÉNIAUT Samuel

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The Councils of use of STAT_NON_LINE

Summary

The objective of this note is to give some advices to a user wishing to carry out nonlinear calculations with *Code_Aster* by using the operator STAT_NON_LINE [U4.51.03].

General advices are initially given. Then one specifies the solutions to be implemented for the principal types of encountered problems. The problems of which it is question are of standard not-convergence, or failure of an algorithm. One also returns towards documentation specific to each problem.

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1   Introduction

The purpose of this document is to help the user to solve a problem of mechanical evolution or thermo-hydro-mechanics, into quasi-static, of a structure into non-linear, *via* the operator STAT_NON_LINE. A detailed presentation of the algorithm of this operator is made in his theoretical documentation [R5.03.01].
The 3 great types of nonlinearities are the following ones:
* non-linearity related to the behavior of material (for example plastic);
* non-linearity related to the geometry (for example in great displacements);
* non-linearity related to contact-rubbing.

In the 2nd part of this document, one details the principal tools which one lays out to help the convergence of calculations and to improve quality of the results. The following parts are devoted to the advices of use. In the 3rd part, one gives general advices, commun runs with the 3 types of non-linearities. In 4th, 5th and 6th parts, one gives advices dedicated to each of the 3 types of non-linearities: materials, then geometrical and finally of contact-rubbing. These advices refer to the tools evoked in 2nd part.

2   Tools of assistance to convergence

In the event of problems, one has several tools:
* under-cutting of the step of time,
* to change the matrices,
* piloting,
* linear research,
* to change finite elements formulation.

2.1   The under-cutting of the step of time

In a general way, plus the step of time is small, less the problem is non-linear, therefore easier to solve. The under-cutting of the step of time is thus an essential tool which makes it possible to pass the most current difficulties. Under-cutting activates by default in DEFI_LIST_INST [U4.34.03]. One advises always to activate it. Moreover, more the step of time is small, and more the error of temporal discretization is small.

2.2   The wise choice of the matrices

In the algorithm of Newton, it is possible to use various matrices in prediction and correction and to more or less often reactualize them. These choices are specified in STAT_NON_LINE under the keyword NEWTON [U4.51.03]. The most general-purpose and robust choice is to use the tangent matrix reactualized with each iteration of Newton and to choose an elastic prediction.

PREDICTION=' ELASTIQUE'
MATRICE=' TANGENTE' (by default)
REAC_ITER=1
REAC_INCR=1 (by default)

In the event of problem of convergence to spend one delicate moment, it can be interesting to rock of the tangent matrix towards the matrix of décahrge if the step of time becomes too small (i.e. when the step of time in question under-was cut out many times successively). The step value of time below which one takes the matrix of discharge is given by the keyword PAS_MINI_ELAS. The frequency of actualization of the matrix of discharge is defined by REAC_ITER_ELAS. For a definition matrix of discharge specifies, to see the keyword factor NEWTON of [U4.51.03]).

2.3   Piloting

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The piloting of the loading is a method of continuation for the method of Newton. Piloting makes it possible in particular to as well calculate the answer of a structure which would have instabilities, of origins geometrical (buckling) as material (softening). Its employment is limited to simulations for which time does not play of physical role, which excludes *a priori* dynamic, or viscous or thermomechanical problems.

2.4 Linear research

The method of Newton provides an increment of the unknown factors, but this increment is valid only in one vicinity of initialization. The idea of linear research is to use the direction of the increment, but by controlling the length of advanced in this direction. The step of advance is then chosen by minimization of a functional calculus. That in particular makes it possible to avoid certain divergences of the algorithm of Newton. However, the activation of linear research is "expensive". It is recommended to activate it only where necessary.

In certain cases, LE choice of partitionnor can have an influence on linear research. One thus advises is to increase ITER_GLOB_MAXI or to change partitionnor. The partitionnor SCOTCH TAPE tends to better behaving than the MONGREL partitionnor in certain cases (CAS-test ssns115b).

2.5 The wise choice of the formulation element-finish

All element-finish them are not worth themselves. Certain elements behave better than others in certain situations [U2.01.10]. The choice of element-finish is made in the operator AFFE_MODELE.

3 The Councils common to the 3 types of non-linearities

In this part, one gives general advices on the resolution of non-linear problems

3.1 Management of the list of moments

The management of the list of moments is specified via the operator DEFI_LIST_INST [U4.34.03]. By default, the under-cutting of the list of moments beT activated in the event of error (in the contact, the law of behavior, piloting, factorization…). It is also possible to start the under-cutting of the step of time when the increment of a size exceeds a fixed threshold (DELTA_GRANDEUR). That makes it possible for example to make sure that an internal variable does not vary too much during a step time. Another possible cause of under-cutting is a not-reduction in the residue during iterations of Newton (DIVE_RESI). That makes it possible under-to cut out in the event of problem without waiting to arrive at the end of the iteration count authorized of Newton.
The management known as manual of the list of moments is classical management: calculation follows the list of moments provided by the user (with possibility of under-cutting). It is also possible to choose an automatic management of the list of moments. In this case, the user gives only a few moments of passages (urgent where the loading changes for example, or moments of postprocessing). According to a first experience feedback, the automatic management of the step of time [bib1]:

- have a real interest if the user is not informed any *a priori* discretization temporal,
- often allows to save a considerable time for the non-linear studies "slightly", i.e. the studies which converge without advanced techniques (piloting, linear research),
- often fail for the non-linear studies "strongly" if it is used only; it appears necessary to combine it with another technique, as linear research.

This operator also allows to extract from a preceding calculation the list of the really calculated moments and to refine it of a factor 2. It is then possible to start again same calculation with this new list 2 times finer in order to control the error due to the temporal discretization.

3.2 Management of the loadings

The application of a loading in effort or displacement imposed not-no one is usually done in a gradual way (by stages of load). For that, it is possible to define a loading of type function (time), or to multiply

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the loading by a function of the type crawls (with `FONC_MULT` under the keyword `EXCIT` of `STAT_NON_LINE`), except in the event of piloting.

The loads being used for the boundary conditions (of standard displacement imposed no one) or with the contact are applied directly and do not require the definition of a function for a gradual application.

3.3   Management of the convergence of the non-linear total algorithm

By default, the algorithm of total resolution non-linear is based on the method of Newton-Raphson. The parameter setting of the convergence of the algorithm of Newton is made under the keyword factor `CONVERGENCE` of `STAT_NON_LINE` [U4.51.03].
The convergence of the algorithm of Newton is characterized by the data of a value threshold of the residue. When the value of the residue is below of this threshold, the algorithm converged. By default, it is the relative residue which is taken into account. The threshold is then given by the keyword `RESI_GLOB_RELA` (10^{-6} by default). **It is strongly to disadvise modifying this threshold of convergence**.
When the imposed loading is null (in the event of total discharge for example), the relative residue does not function and one tries to pass automatically to absolute convergence criteria (`RESI_GLOB_MAXI`). This operation is transparent for the user. In a general way it is disadvised informing `RESI_GLOB_MAXI`. When these convergence criteria are not enough, it is possible to use finer criteria: a criterion which reasons component by component (`RESI_COMP_RELA`) or a criterion which reasons starting from a value of reference for each quantity (`RESI_REFE_RELA`).

3.4   Management of filing

The question of the filing of the computed fields into implicit is a question less important than in explicit dynamics, where the number of steps of time is generally very high.

According to the size of storage which one lays out, and the number of fields which one wishes to store, it is possible to evaluate the number of steps time that one be able to store.
By defaults, all the steps of time are filed, including the moments of calculations lately created by automatic recutting of the step of time. As this number cannot be given in advance, it is advised to file only the moments of the initial list of moments. If this list still contains too many moments, it is advised to create one 2ème list, reduced, specific to filing. If the initial list of moments contains many moments and that the automatic under-cutting of the step of time is not activated (it is not advised), one can also limit filing by a frequency of filing.

It is also possible to reduce the obstruction of the structure of data `result` by extracting certain fields (operator `EXTR_RESU`).

3.5   Observation and followed by certain sizes

It is possible to store in a table certain components of the computed fields on parts of the model at moments of a list (known as of observation) generally finer than the list of the filed moments. This functionality can be activated in `STAT_NON_LINE` under the keyword `OBSERVATION`. That makes it possible to reduce the needs for filing considerably. However, it is advisable to be careful in the use of the observation. Indeed, this functionality was conceived for some points in the structure and it is not advised to make several thousands of observations to each step of time, for reasons of performance.

It is also possible to follow the evolution of certain components of the computed fields during iterations of Newton and to display them in the table of convergence. This functionality can be activated in `STAT_NON_LINE` under the keyword `SUIVI_DDL`.

3.6   Posting of information and performance

Many information is displayed by default in the files message and results (`.mess` and `.resu`).

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Essential information is the table of convergence displayed at every moment of calculation. This table is very useful and in particular makes it possible to identify certain anomalies of convergence.

The operator STAT_NON_LINE poster size of the matrix (many equations of the system).
According to the size of the matrix, the use of an iterative solvor (like PETSC) a saving of time will allow. For information, it is considered that an iterative solvor is faster than a direct solvor (by default) starting from approximately 200 000 equations in 3D. The counterpart of the use of an iterative solvor is an unguaranteed robustness. It should be noted that the use of PETSC require a version MPI of *Code_Aster* (even if one uses one processor).

The use of parallelism can be also effective if the time spent in STAT_NON_LINE is dominating compared to the total time of calculation. For that, it is enough to choose an adequate solvor (example: MUMPS , PETSC), a version MPI of *Code_Aster* and to specify the number of processes in Astk. Many advices on parallelism are given in the document [U2.08.06]. Finer information over the times spent in each part of the resolution is also displayed, and can be used for better parameterizing calculation (time, memory, number of processor…). One returns for that to documentation [U1.03.03].

4   Non-linearity material

This part deals with problems most frequently met during the use of non-linear laws of behaviors.

4.1   Parameter related to the resolution of the behavior

Most laws of behavior of *Code_Aster* be integrated in an analytical way. In the event of error in the integration of the law of behavior, there is thus no digital parameter which one can exploit. The usual solution consists in Re-cutting out the step of total time (or to choose a finer list of moments).
Certain laws of behavior are solved locally via an iterative digital method, for which the user can choose the authorized maximum residue and the iteration count local maximum. Most of the time, the parameters by default (RESI_INTE_RELA = 10^{-6} and ITER_INTE_MAXI = 20) are enough. In the event of error in the integration of the law, one can like previously under-cutting out the step of time, but also authorizing local iterations moreover (ITER_INTE_MAXI). For example, for MONOCRYSTAL, it is frequent to authorize 100 or 200 local iterations. The choice of the residue is more delicate. Indeed, it is important that the behavior is correctly integrated. That means that it is imperative not to increase the residue beyond the value by default (10^{-4} for example), except for the behaviors integrated by an explicit algorithm. On the other hand, it is sometimes advised to tighten the residue (for example RESI_INTE_RELA = 10^{-10}). In fact, according to the way in which the behavior is implemented, the residue does not have the same physical meaning (forced, deformation…). It is then necessary to refer to the reference material of the law of behavior in question.

4.2   Management of the plastic incompressibility

If the material is incompressible ($\nu > 0.45$) or in the event of strong plastic deformations, of the oscillations on the constraints or on the trail of constraints can appear. Certain finite elements spéciauX, like the under-integrated elements or the mixed elements, make it possible to deal with these problems [U2.01.10]. If the use of under-integrated elements does not solve the problem, then one advises the use of the formulatione mixed with 2 fields (displacement and pressure) in small deformations and of the mixed formulation with 3 fields in great deformations. To note that the latter functions only on quadratic grids.

4.3   Discharge

In the event of discharge, one can encounter problems of convergence of the algorithm of Newton. One advises to use the elastic prediction (in STAT_NON_LINE under the keyword NEWTON). It is also useful to activate the under-cutting of the step of time in the event of singular matrix (it is automatic in version 11, but to activate with the hand in the previous models *via* STOP_SINGULIER = 'CUTTING' in STAT_NON_LINE under the keyword SOLVEUR).

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4.4 Plane constraints

The treatment of the condition of plane constraints is carried out within the framework general by the method of Deborst. It is advised to often reactualize the tangent matrix (all the one with three iterations of Newton). In certain cases, convergence is reached for the algorithm of Newton, but not for the checking of the state of plane stresses, which leads to additional iterations, even an excessive recutting of the step of time. It is then advised to activate an additional loop for better satisfying the plane constraints during iterations with Newton: ITER_CPLAN_MAXI must be selected at least equal to 5 [U4.51.11].

4.5 Damage (lenitive problems)

To deal with the problems of damage, of many advices are given in [U2.05.06]. In a general way, one advises to use piloting, with possibly mixed linear research.

For certain laws of behavior (ENDO_FRAGILE and ENDO_ISOT_BETON), method IMPLEX is proposed in alternative of the method of Newton. One activates this method in STAT_NON_LINE under the keyword NEWTON. This method is based on an explicit extrapolation of the internal variables to determine displacements from which the behavior is integrated implicitly. The nullity of balance is not checked. So it introduces an approximation of the resolution but makes it possible to guarantee the robustness of calculation. A control of the error and an optimization of the steps of time are possible via the operator DEFI_LIST_INST by choosing an automatic management of the step of time and a way of calculating of the step of time specific to IMPLEX. From a practical point of view, the method imposes a reactualization of the matrix on each increment and only one iteration. Before any use of the method IMPLEX, the document [R5.03.81] must imperatively be consulted.

4.6 Thermo-Hydro-mechanics (THM)

The problems of THM utilize quite particular concepts. One advises to consult documentation [U2.04.05]. One gives here some general advices for the resolution. The initialization of fields is a delicate stage for which it is necessary well to pay attention (ETAT_INIT). It is necessary to use the reactualized tangent matrix. In the event of problem of convergence, it can be very useful to activate linear research (mixed preferably). Linear research does not improve however systematically convergence, it is thus to handle with precaution insofar as it can increase cost CPU.

5 Geometrical non-linearity

This part deals with problems most frequently met during calculations with geometrical non-linearities.

5.1 Buckling

The operator STAT_NON_LINE allows to calculate a criterion of stability *via* the keyword CRIT_STAB=_F (TYPE=' FLAMBEMENT'). The documentation of use of buckling [U2.08.04] gives many advices on the installation of a calculation of stability. Some general advices here are given.
In a general way, the analysis of stability is led on matrices of reactualized stiffnesses. In practice, it is necessary to limit the calls to CRIT_STAB for reasons of costs of calculation, by limiting the moments over which the analysis of stability is carried out. In complement, it is judicious not to use CRIT_STAB that on the time intervals where one suspects the possibility of instabilities. It is also advisable to refine well the step of time to the approach of this zone. By default, one calculates 3 critical loads (NB_FREQ). Often the first can be enough. One of the particular points related to instability is the choice of the technique of piloting of the algorithm. Indeed, classical piloting in effort is not adapted. For the approach of a boundary point, it is necessary to reduce the increment of load and to increase the maximum number of iterations. It is also advised to use piloting by length of arc.

5.2 Great deformations

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The keyword DEFORMATION under BEHAVIOR allows to define the assumptions used for the calculation of the deformations. By default, one considers small displacements and small deformations. (DEFORMATION = 'SMALL'). That means that one remains in Assumption of the Small Disturbances: small displacements, small rotations, small deformations (lower than approximately 5%). When this assumption is not checked any more, it is necessary to change model of deformations. For the slim structures (hulls, plates, beams), it frequently happens that one is in great displacements, great rotations but small deformations. One uses then DEFORMATION = 'GROT_GDEP'.

The treatment of the great deformations differs according to the type of element and the law from behavior. The model of great deformations of Simo and Miehe (DEFORMATION = 'SIMO_MIEHE') is advised for the relations of behavior VMIS_ISOT_LINE, VMIS_ISOT_TRAC, ROUSSELIER and all the behaviours with isotropic work hardening only, associated with an undergoing material of the metallurgical phase shifts (relations META_X_IL_XXX_XXX and META_X_INL_XXX_XXX). For the other laws of behavior, one advises the model of great deformations of Miehe and Apel (DEFORMATION = 'GDEF_LOG'), theoretically applicable to any law of behavior for modelings 3D and 2D. More detailed explanations are in the note of use of the non-linear behaviors [U4.51.11] in the paragraph DEFORMATION.

6   Non-linearity of contact-rubbing

The definition of the load of contact-rubbing been the object of a specific operator: DEFI_CONTACT [U4.44.11]. In addition to the choice of the entities in contact, this operator allows to choose the type of formulation of the problem of contact (discrete or continues), of the parameters for the operation of pairing and of the parameters for the phase of resolution. Many advices of setting in data are available in the document [U2.04.04], in particular on the choice of surfaces main and slave.

The taking into account of the conditions of contact with or without friction led to non-linear problems, which can cause difficulty in the resolution of STAT_NON_LINE. One of the first difficulties is the blocking of the rigid modes of body. Indeed the conditions of contact-rubbing do not intervene in the scrap-metal of the rigid modes. It is thus necessary to block the rigid modes without taking account of the conditions of contact (except rare exceptions). A bad blocking of the rigid modes of body involves the appearance of worthless pivots during the factorization of the matrix. Advices are given in documentation [U2.04.04]. Attention, certain formulations of contact require a particular solvor. In particular, in discrete formulation, the method CONSTRAINT require a direct solvor (MULT_FRONT or MUMPS). In a general way, one disadvises the use of linear research with the contact. In the event of coupling with other non-linearities, it is advised to make sure that each taken non-linearity separately converges. So problems appear only when non-linearities are coupled, it is advised to work with the reactualized tangent matrix and an elastic prediction.

A comparative benchmark enters *Code_Aster* and other commercial software was carried out in 2010 on 5 problems of contact-rubbing [2]. This benchmark in particular made it possible to highlight oscillations of the contact pressure for the formulation continues in the event of incompatible grids, defect from which also the commercial software used suffers. It is then recommended to extract contact pressures starting from the constraints on the edge, or to use compatible grids.

7   Bibliography

[1]   S. Geniaut, First REX on the automatic management of the step of time in STAT_NON_LINE, CR-AMA-09.268, 2009

[2]   T. De Soza, Assessment of the batch "Contact/Friction" in 2010 (project MNAM), CR-AMA-11.049.2011