

The Councils of implementation of non-linear calculations

Summary

The objective of this document is to give advices to a user wishing to carry out non-linear calculations with *Code_Aster*. The user of linear calculations will find there also useful information and advices.

The aspects according to will be approached:

- grid and modeling,
- loadings and boundary conditions,
- materials and laws of behavior,
- non-linear resolution,
- management memory/time and optimization,
- control of the error and quality.

This document does not treat questions specific to dynamics.

1 Grid and modeling

The choice of the finite elements influences directly the solution. By choice, one hears the choice of the degree of the approximation element-finish as well as the choice of a formulation. The degree of the approximation being generally connected to the degree of the meshes, the paragraphs according to treat choice of the degree of the grid and the choice of a formulation element-finish, with a particular point for the problems of incompressibility.

1.1 General information on the choice of the degree of the grid and the choice of the finite elements

In a general way, the use of a linear grid is advised in thermics and the use of a quadratic grid is advised in mechanics. The order `CREA_MALLAGE` (`LINE_QUAD` and `QUAD_LINE`) allows to pass from a linear grid to a quadratic grid and vice versa, but does not allow to generate quadratic elements on curved board. It is preferable besides to directly generate the quadratic elements with the tool for grid (the module of grid of Salomé-Meca for example). For the breaking process, the use of elements of Barsoum in bottom of crack improves quality of the result (order `MODI_MALLAGE / NOEUD_QUART`).

The choice of the finite elements is carried out in the order `AFFE_MODELE`. In thermics, it is advised to use lumpés elements (`_DIAG`). In mechanics, the finite elements classically used are the isoparametric elements (`3D`, `D_PLAN`, `C_PLAN`, `AXIS`). However, these elements are badly adapted to the quasi-incompressible problems. The choice of a formulation answering this problem is the object of the following paragraph.

For more details, to see [\[U2.01.10\] "Note of use on the choice of the finite elements"](#)

1.2 Choice of a formulation to deal with the quasi-incompressible problems

A problem is quasi-incompressible if the Poisson's ratio is close to 0.5 ($\nu > 0,45$) or if the rate of plastic deformations is high. That results in an oscillation of the trace of the constraints. There exist 6 formulations to deal with this problem in *Code_Aster* whose choice depends on the type of meshes, of the model of deformation and the ratio quality/cost calculation.

The possible formulations are:

- in small deformations: `_SI`, `_INCO_UP`, `_INCO_UPG`, `INCO_UPO`
- in great deformations: `_INCO_UP`, `_INCO_UPG`.

All the formulations are compatible with modelings `3D`, `D_PLAN` and `AXIS` but in plane constraints (`C_PLAN`) only the under-integrated formulation (`_SI`) is possible.

The table below has compatibility between quasi-incompressible and standard formulation of meshes (limited to the principal meshes 3D).

	_SI	_INCO_UP	_INCO_UPG	_INCO_UPO
HEXA20	X	X	X	
PENTA15		X	X	
PYRAM13				
TETRA10	X	X	X	
HEXA8	X			X
PENTA6				X
PYRAM5				X
TETRA4		X		X

In the case general, it is thus necessary to mix various formulations to cover all the types of meshes (for example, as no formulation manages the meshes `PYRAM13`, it is also necessary to affect an isoparametric modeling).

If one remains in small deformations, it is advised to use a mixture of formulations (grid which can comprise several types of meshes):

	quality	cost
MODELISATION= ('3D', '3D_INCO_UPG', '3D_INCO_UPO')	+++	+++
MODELISATION= ('3D', '3D_INCO_UP', '3D_INCO_UPO')	++	++
MODELISATION= ('3D', '3D_SI', '3D_INCO_UPO')	+	+

For more details, to see [\[U2.01.10\] "Note of use on the choice of the finite elements"](#)

2 Loadings, boundary conditions, conditions initial

2.1 Heart of the problem

The loadings and boundary conditions are important for a good modeling. Their influence on the results is most of the time direct, so that one can check their application by a simple preliminary calculation, for example using `MECA_STATIQUE`, or by visualizing the boundary conditions *via* the keyword `CONCEPT` of `IMPR_RESU` with the format `MED`.

With regard to the boundary conditions, it is often a question of introducing the minimum of it to block displacements of rigid solid, therefore to avoid having floating bodies in the structure, which would cause a null pivot or a singular matrix at the time of the resolution.

Certain boundary conditions are non-linear, for example the unilateral contact. Their checking cannot thus be made using the first linear calculation (`MECA_STATIQUE`): the various objects in contact should not have rigid movement of body [U2.04.04] [Note of use of the contact](#). If it is the case, one can to avoid the worthless pivots by adding discrete elements (springs) of low rigidity.

The loadings (other that blockings) can consist either of imposed conditions of displacement, or in imposed efforts, or of standard imposed initial field.

In all the cases, it is important to represent reality well. One will be able to use with profit the conditions of symmetry or antisymmetry [1].

In a general way, a condition of type imposed displacement does not provide the same results as a condition of the type forces imposed: a displacement imposed on part of the border imposes that displacement (imposed) is constant spaces some on this part, therefore brings rigidity, even of the singularities. Let us take the example of the punching of a solid mass: the displacement imposed on the edge of the induced punch of the singularities of constraints of comparable nature that those which are met at the bottom of a crack.

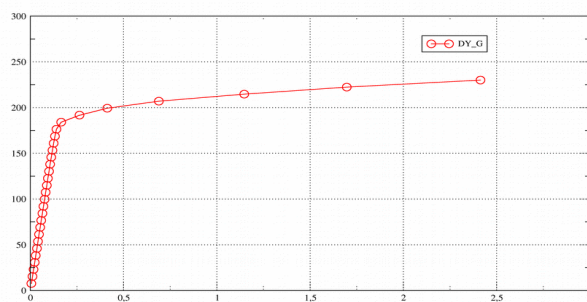


Figure 2.1-1: Example of curved force-displacement

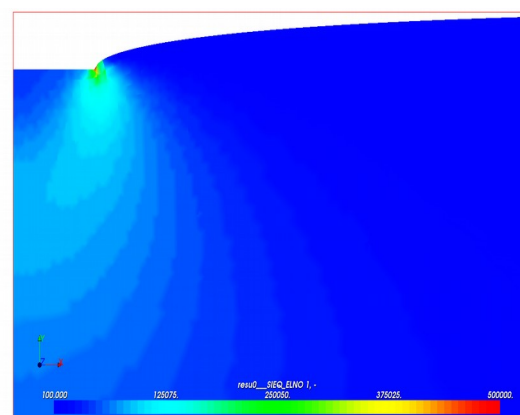


Figure 2.1-2: punching with imposed displacement

Moreover, for nonlinear calculations, the control of calculation is not the same one: in the event of softening or of limiting load, the loading with imposed force can be illicit (beyond the limiting loading). Let us take for example punching (see Figure 2.1-1 and Figure 2.1-2): the answer in terms of resulting force on the punch according to displacement shows that the more the imposed force approaches the limiting load, the more convergence will be difficult, until being impossible beyond the limiting load. If correct modeling requires to apply an imposed force, the problem can be solved *via* the piloting of the force imposed compared to the displacement of a point or a set of points (method of continuation or length of arc) (see [R5.03.80] [Methods of piloting of the loading](#)).

Documentations of use relating to the application of the loadings and boundary conditions are [\[U4.44.01\] AFFE_CHAR_MECA](#) and [\[U4.44.03\] AFFE_CHAR_CINE](#).

2.2 Precautions for the application of the loadings

It is useful for the application of the loadings to traverse the various keywords of [\[U4.44.01\] AFFE_CHAR_MECA](#). Attention with the vocabulary, in particular, loadings of the type `FORCE_FACE`, `PRES_REP`, `FORCE_CONTOUR`, `FORCE_ARETE`, `FORCE_INTERNE`, `FORCE_COQUE`, `FORCE TUYAU` correspond to forces distributed (linear, surface, voluminal) and **are expressed in unit of constraints** (for example of Pa in unit S.I). Only them `FORCE_NODALE` are expressed in unit of forces (N), and forces distributed of beams (`FORCE_POUTRE`) in units of force divided by a length.

With regard to the pressures (`PRES_REP`, `FORCE_COQUE/PRES`), the pressure applied is positive according to the contrary direction of the normal to the element. It is strongly advised to reorientate these normals *via* the operator `MODI_MALLAGE`, keywords `ORIE_PEAU_*`, `ORIE_NORM_COQUE`.

For the continuous mediums 2D, 3D, the use of specific forces (`FORCE_NODALE`) is to be proscribed, because it always involves singularities.

The application of loads function of time can be carried out in two ways:

- maybe by defining constant loads, then by applying a multiplying coefficient function of time to these loads at the time of the resolution (keyword `FONC_MULT` under `EXCIT` in `STAT_NON_LINE`),
- maybe by directly defining loads function of time via `AFFE_CHAR_MECA_F`.

If the loadings are of imposed displacements type, those can be introduced either by `AFFE_CHAR_MECA (_F)`, that is to say by `AFFE_CHAR_CINE (_F)`. The use of this last order allows a time-saver calculation which can be appreciable into non-linear (because she does not add multipliers of Lagrange, there are thus less equations to solve).

The variables of orders are not part of the orders `AFFE_CHAR_MECA (_F)`. They are however, in many modelings, comparable to loadings: for example thermal dilation can with it only generate stress and strain states leading to non-linearities of behavior. The variables of orders are applied via `AFFE_MATERIAU`.

It is necessary however to announce here a precaution of modeling concerning these variables of order: indeed, as soon as calculation is incremental, `STAT_NON_LINE` use with each step of time the increment of variable of order to calculate the corresponding deformations (cf for example [\[R5.03.02\] Integration of the relations of elastoplastic behavior of Von Mises](#)). In general, it preferable that at the initial moment, the structure is not forced, not is deformed. If it is not the case, it is necessary to add one preliminary moment where the structure is at rest, to see for example the test `FORMA30` [\[V7.20.101\] FORMA30 - Hollow roll thermoelastic](#). In the event of detection of constraints due to the variables of orders at the initial moment one obtains alarm:

<A> <MECANONLINE2_97>:

- > the variables of initial orders induce incompatible constraints:
the initial state (before the first moment of calculation) is such as the variables of order (temperature, hydration, drying...) lead to not balanced constraints.

- > Risk & the Council: in the case of an incremental resolution, one considers only the variation of the variables of order between the previous moment and the current moment. One thus does not take into account possible incompatible constraints due to these initial variables of order.

To take account of these constraints you can:

- to start from one former fictitious moment where all the variables of order are worthless or equal to the values of reference
- to choose adapted values of reference

For more information, to see the documentation of `STAT_NON_LINE` (U4.51.03) keyword `EXCIT`, and test `FORMA30` (V7.20.101).

2.3 Various types of boundary conditions

The boundary conditions simplest are mainly used to introduce conditions of symmetry, on the one hand, and to prevent the movements of rigid solid, on the other hand. When they are of standard imposed degree of freedom, one can use is `AFFE_CHAR_MECA`, that is to say (to optimize time calculation) `AFFE_CHAR_CINE` [\[U2.01.02\] Note of use of the boundary conditions treated by elimination](#).

A methodological council: it is always preferable to rather apply the boundary conditions to groups of meshes than to groups of nodes or lists of nodes or meshes. Indeed, the groups of meshes correspond to geometrical zones, and are preserved at the time of a refinement of the grid (manual or using Lobster), whereas the groups of nodes are modified. This is why in `AFFE_CHAR_MECA` the keyword `DDL_IMPO`, `FACE_IMPO`, `LIAISON_UNIF`, like all the keywords of `AFFE_CHAR_CINE` comprise the keyword `GROUP_MA`, to thus privilege.

It is sometimes necessary to impose linear relations between degrees of freedom. Keywords `LIAISON_*` of `AFFE_CHAR_MECA` allow to introduce this kind of relation. The elementary relations can be defined using `LIAISON_DDL`, but that becomes tiresome if them equations to be written are numerous. Features moreover high level are available, for example:

- `LIAISON_SOLIDE` to rigidify part of the structure, (in small deformations and small displacements only) [\[R3.03.02\] Conditions of solid connection of body](#) ;
- `LIAISON_UNIF` to ensure that part of the border will keep same displacement (unknown a priori); [\[U4.44.01\] AFPE_CHAR_MECA](#)
- `LIAISON_MAIL`, `LIAISON_GROUP` to connect two edges,
- and other specific keywords of `AFFE_CHAR_MECA`.

Moreover it is possible to connect (to the energy direction) modelings of different nature, via `LIAISON_ELEM` and several options (in small deformations and small displacements only)

- `'2D_POU'`, `'3D_POU'`, beams or discrete with elements 2D or 3D [\[R3.03.03\] Connections 2D-beam and 3D-beam](#);
- `'COQ_TUYAU'`, `'3D_TUYAU'`, elements pipe with plates and hulls, 3D;
- `'COQ_POU'`, beams or discrete with plates and hulls [\[R3.03.06\] Connection hull-beam](#).

Notice : in certain cases, boundary conditions or loadings of type displacement imposed are not appropriate because they bring local rigidity too much. It can be interesting to replace these conditions by a connection between the part of the border concerned and a discrete element, to which will be applied the imposed conditions of displacement or a torque of imposed efforts. That means that displacements of the border will be equal on average to the displacement of the discrete element, without introducing secondary stresses. On the other hand, this process introduces additional degrees of freedom (multiplying of Lagrange), the resolution of the linear systems can thus be more expensive.

The unilateral contact, with or without friction, is a kind of boundary conditions individual. It is strongly nonlinear, and its treatment in `STAT_NON_LINE` / `DYNA_NON_LINE` require additional iterations to obtain convergence. It is strongly advised to consult the document [\[U2.04.04 Note of use of the contact\]](#) to model correctly these phenomena.

2.4 Initial conditions

In `AFFE_CHAR_MECA`, it is possible to define loadings of average deformations or average constraints, overall uniform (keywords `PRE_EPSI`, `PRE_SIGM`).

One should not confuse these loadings and the strains and initial stresses used into nonlinear, because these quantities do not intervene directly in the expression of the law of behavior, but only with the second member.

The stress fields, displacements and variable internal initial are to be provided directly in `STAT_NON_LINE` (keyword `ETAT_INIT`). To build these fields, it can be useful to consult it document [\[U2.01.09\] analytical Definition of a stress field and a field of internal variables initial](#).

3 Materials and behaviors

3.1 Choice of the law of behavior

The choice of the law of behavior is of course function of the material which one models, but also phenomena to be treated: for example, the same steel will be elastoplastic at low temperature, and viscoplastic at high temperature. Values of the parameters of these laws (in `DEFI_MATERIAU`) are often identified in a range of deformation, speed, temperature quite specific.

- For the elastoplastic behaviors, to see [\[U2.04.03\] Choice of the behavior élasto- \(visco\) - plastic](#)
- For the laws with damage (case of the concrete for example), to see [\[U2.05.06\] Realization of calculations of damage into quasi-static](#)
- Pour metallurgy, to see [\[U2.03.04\] Note of use for calculations thermometallomecanic on steels](#)
- Pour porous environments in THM, to see [\[U2.04.05\] Note of use of model THM](#) and [\[R7.01.11\] Model of behavior THHM](#)
- For the use of elements CZM, to see [\[U2.05.07\] Note of use of the models of cohesive zones](#)

3.2 Keywords of BEHAVIOR

3.2.1 DEFORMATION

This keyword makes it possible to define the assumptions used for the calculation of the deformations: by default, one considers small displacements and small deformations. The type of deformation used can have a great influence on calculation as soon as a component of the deformations exceeds a few % (typically 5%).

- **SMALL** : small deformations, small displacements. Linearity of the operator deformation.
- **GROT_GDEP** : allows to treat great rotations and great displacements, but while remaining in small deformations. This is particularly useful for the slim structures (modelled in beams, hulls, or 3D) and the study of buckling (see for example the test [\[V6.02.134\] SSNL134 - Ruin elastoplastic of the gantry of Lee](#)).

With regard to the laws very-rubber bands of the type `ELAS_VMIS`, they are not adapted with the great deformations (loss of existence of the solution, to see the §2,1 of [\[R5.03.20\] Relation of nonlinear elastic behavior in great displacements](#)). It is necessary to use is a model great deformations with `VMIS_ISOT`, that is to say the behavior `ELAS_HYPER`.

- **GDEF_LOG** : model of great deformations, using a measurement of deformation logarithmic curve, and which makes it possible to use elastoplastic laws of behaviour to isotropic or kinematic work hardening (see the list of the behaviors in [\[U4.51.11\] nonlinear Behaviors](#)). The relation stress-strain being hypo-rubber band, this formulation is limited to the weak elastic strain (but great plastic deformations).
- **SIMO_MIEHE** : model of great deformations of the laws of behaviors being based on a criterion of Von Mises with isotropic work hardening, and all the behaviours with isotropic work hardening associated with an undergoing material of the metallurgical phase shifts. The relation stress-strains rubber band is very-rubber band, which makes it possible to treat the great elastic strain (for little that has a direction for material used).
- other formulations exist, to see [\[U4.51.11\]](#).

3.2.2 ALGO_INTE , ITER_INTE_MAXI , RESI_INTE_RELA , ITER_INTE_PAS

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Allows to specify the type of diagram of integration to solve the equation or the system of non-linear equations formed by the equations constitutive of the models of behavior to internal variables. A method of by default resolution is planned for each behavior. However, it is possible to modify the method of by default resolution for a certain number of behaviors (see [\[U4.51.11\]](#)).

In the case of an iterative resolution (i.e. if `ALGO_INTE` is not `ANALYTICAL`), keywords `ITER_INTE_MAXI` and `RESI_INTE_RELA` the maximum number of iterations and the relative residue define to integrate the behavior. If this integration fails, it is possible to subdivide the step of time, that is to say locally (keyword `ITER_INTE_PAS`) that is to say overall (order `DEFI_LIST_INST`). The value by default of `ITER_INTE_MAXI` is 20. That can be insufficient for certain behaviors (`MONOCRYSTAL` for example). Not to hesitate in this case to increase this parameter (100 for example). On the other hand it is strongly disadvised increasing `RESI_INTE_RELA` (10^{-6} by default), under penalty of obtaining not converged solutions.

The local subdivision of the step of time is average to improve the robustness of local integration, on the other hand it does not make it possible to provide a coherent tangent matrix (loss of the quadratic convergence of the total problem).

3.2.3 `POST_ITER=' CRIT_RUPT '`

Definition of a criterion of rupture in constraint criticizes in postprocessing of the iterations of Newton, with each step of time. If the greatest average principal constraint in an element exceeds a given threshold σ_c , the Young modulus is divided with the step of time following by a coefficient. These two coefficients are defined under the keyword `CRIT_RUPT` of the operator `DEFI_MATERIAU`.

3.2.4 `RESI_RADI_RELA`

Measurement of the error due to the discretization in time, directly connected to the rotation of the normal on the surface of load. One calculates the angle between the normal with the criterion of plasticity at the beginning of the step of time and the normal with the criterion of plasticity calculated at the end of the step of time. The step of time is cut out (via `DEFI_LIST_INST`) if the error is higher than the tolerance defined by the user.

This criterion is operational for the elastoplastic behaviors of Von Mises with work hardening isotropic, kinematic linear and mixed and for the behaviors élasto-visco-plastics of Chaboche.

4 Non-linear resolution

3 great types of non-linearities in *Code_Aster* are the following:

- 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.

The general advices of resolution of non-linear problems are the object of a specific document which one strongly recommends the reading: [\[U2.04.01\]](#) “the Councils of use of `STAT_NON_LINE`”.

Before any non-linear calculation, it is essential to make sure that calculation functions correctly in linear elasticity. Non-linearities could then be added the ones after the others.

One briefly recalls the major advices on the temporal discretization and the digital parameters of non-linear resolution in the following paragraphs.

4.1 Non-linearity and temporal discretization

The resolution of a non-linear problem generally requires to apply the external loading gradually, by increment of load. Thus time (or pseudo-time into quasi-static) is discretized in step of time and to each step of time an increment of load corresponds (to see §2.2). The smaller the step of time is, the less the problem is non-linear thus easier to solve. In order to authorize the under-cutting of the step of time in the event of failure of convergence, it is essential to use the order `DEFI_LIST_INST` (for more details on management of the list of moments, to see the paragraph §3.1 document [\[U2.04.01\]](#))

To check the coherence of the data (system of units, boundary conditions, characteristics elementary, effect of the variables of orders), it is always useful to carry out a first linear elastic design (`STAT_NON_LINE/RELATION=' ELAS '`, or `MECA_STATIQUE`), before any nonlinear study, then to add nonthe linearities ones after the others.

4.2 Digital parameters for the non-linear algorithm of resolution

By default, the non-linear algorithm of resolution is based on the method of Newton-Raphson (`STAT_NON_LINE/METHODE=' NEWTON '`).

It is advised to use a tangent matrix reactualized with each iteration of Newton: `REAC_ITER=1` in order to facilitate the convergence of the algorithm (see the paragraph §2.2 document [\[U2.04.01\]](#)).

It is strongly recommended not to increase the convergence criteria of the method of Newton (`RESI_GLOB_RELA=10-6` by default). Other convergence criteria are also available (see the paragraph §3.3 document [\[U2.04.01\]](#)).

Note:

- For lenitive problems, *Code_Aster* offer the possibility of using an alternative method with the method Newton-Raphson: it is the method `IMPLEX` who is a robust but approximate method (see the paragraph §4.5 document [\[U2.04.01\]](#)).
- For an optimization of the computing time, *Code_Aster* offer the possibility of using an inaccurate method of Newton (provided that the selected linear solver is an iterative solver): it is the method `NEWTON_KRYLOV`.

5 Management memory/time and optimization

Before speaking about optimization, the first question which one installation is how to choose the parameters of execution in `Astk`: total memory and time so that the first launching of calculation finishes correctly. Then, once calculation will have passed for the first time, it will be always possible to try to optimize it according to information which one will have recovered of the 1^{er} calculation.

5.1 First execution of a calculation

The knowledge of the memory size which one lays out is necessary. The answer depends of course on the object computer: centralized waiter, local machine.... On a local machine, it is always possible to authorize the maximum memory available whereas on the centralized waiter, it can be convenient not to ask too much memory under penalty of having to wait until the associated class of job is released.

Estimate of the memory necessary : into quasi-static, the total memory is generally function of the size of the linear systems to solve. For the isoparametric finite elements, it is rather easy to consider the size total of these systems. The number of degrees of freedom can be estimated by the relation: (many nodes of the grid) X (dimension of the problem (2 or 3))

This relation does not take into account the ddls relating to the boundary conditions dualized. But generally, this share is weak. If the finite elements are not isoparametric (mixed formulations for example), this estimate is more delicate.

In any case, the size of the linear systems is displayed with each resolution in the file `.mess : full number of equations` or the matrix is of size `N equations`. It is **important to know this number** (although with him only, it is not always a completely reliable indicator, because the memory and the time necessary with the resolution of a linear system depend on good of other parameters: size of the bandwidth, many nonworthless terms in the matrix, renumerator... but that would take us along too far). Thus if one cannot estimate the size of the linear system, it is interesting of **for the first time to launch the study in degraded mode** : reading of the grid, assignment of element-finish, material and resolution (`MECA_STATIQUE` or `STAT_NON_LINE`) with the direct solver `MUMPS`. To launch the study simplified in interactive mode with interactive follow-up, then to once stop calculation information on the known size of the system.

In the ideal¹, it is necessary to have approximately 30 Go to make pass a calculation to a million degrees of freedom (case of the cube with a grid in `HEXA8`, of which a face is embedded by dualisation), minimal memory² being 9 Go. The table below gives orders of magnitude of the "ideal" memory (or optimal) and minimal to solve a system of size given (with the direct solver `MUMPS`).

Many degrees of freedom	Minimal memory	"Ideal" memory
200000	1 Go	4 Go
400000	2.5 Go	9 Go
600000	4 Go	15 Go
800000	6 Go	23 Go
1000000	9 Go	31 Go

Once the estimated necessary memory, one can launch complete calculation with direct solver `MUMPS`. Following this 1^{er} calculation, it is very interesting to look at:

- In the file `.mess` total memory (`JEVEUX + python + external bookstores`) used by calculation: this information is displayed at the end of the file: to see `MAXIMUM OF MEMORY UTILISEE BY THE PROCESS` ;

¹ Ideal wanting to say management of memory here `IN_CORE`

² Minimal wanting to say here for a management `OUT_OF_CORE`

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- In the file `.resu` : the time of resolution (MECA_STATIQUE / STAT_NON_LINE) compared to the total time of calculation.

5.2 Optimization of a calculation

The optimization of a calculation on the aspects time and memory is an interesting operation but a little delicate because there does not exist miraculous formula. Moreover it is not always easy to make the distinction between optimization of the memory and optimization of the computing time, therefore in the following paragraphs, one gives tracks of optimization “in the broad sense” and one returns towards the adequate documents.

Parallelism

The use of parallelism is certainly the easiest solution and surest to decrease the computing time (and sometimes also memory necessary). Parallelism consists in carrying out operations on several processors at the same time. The installation of parallelism is effective only 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 solver (example: MUMPS, PETSC), a version MPI of Code_Aster and to specify the number of processors in `Astk` (finely Options/`mpi_nbcpu`). On the centralized waiter `aster4`, one advises to start by choosing `mpi_nbcpu=2`, to observe the saving of time then to start again with `mpi_nbcpu=4`, then possibly `mpi_nbcpu=8`. It is possible to choose `mpi_nbcpu=16` but one is likely to wait a long time before all these processors are available, therefore before calculation starts (all depends on the load machine!).

Many advices on parallelism are given in the document [\[U2.08.06\] “Note of use of parallelism”](#). 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, many processors...). One returns for that to documentation [\[U1.03.03\] “Indicating of performance of a calculation \(time/memory\)”](#).

The linear solver

According to the size of the matrix, the use of an iterative solver (like PETSC) instead of a direct solver a saving of time will allow. For information, it is considered that an iterative solver is faster than a direct solver (by default) starting from approximately 200 000 equations in 3D. But that depends on the type of structure³. The counterpart of the use of an iterative solver 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). From a certain size of problem (a few million ddls), the use of a direct solver becomes impossible and it is essential to use an iterative solver.

In the event of failure of the resolution by an iterative solver, the levers of actions are the choice of another preconditionnor (direct preconditionnor single precision by default `LDLT_SP`, incomplete preconditionnor `LDLT_INC`,...), the choice of another iterative algorithm (`GMRES` by default, `CG`, `CR`, ...).

Many advices on the choice of the solver are given in [\[U2.08.03\] “Note of use of the linear solveurs”](#).

The management of the total base

In the event of going beyond the limiting memory, one can exploit the filing of the results. Filing (keyword factor `FILING` of `STAT_NON_LINE`) allows to appreciably reduce the size of the bases by selecting the saved moments. By default, all is filed (even moments resulting from the under-cutting of the step of time). In the phase of installation of a study, that can prove to be useful, but too expensive in memory. The observation and the follow-up of certain sizes can meet the need for filing efficiently (see §3.4 [\[U2.04.01\] “the Councils of use of STAT_NON_LINE”](#)). Once the study installation, one can restrict filing with a limited number of steps of time (urgent of postprocessing for example).

To reduce the obstruction of the structure of data `result`, it is possible to choose a *posteriori* fields to be filed either by indicating the fields to be preserved, or by indicating the fields to exclude (order `EXTR_RESU`). The extraction can also be done on part of the grid or model. The order `TO_DESTROY` can also be used to destroy a concept. Following these operations of extraction or suppression, it is necessary to specify `RETASSAGE=' OUI '` in the order `END` in order to recover the disk space indeed associated with the total base.

To reduce the size of the files `result` to format `MED` (`.rmed`): to use `IMPR_RESU/RESTREINT`.

³ A cube is penalizing for the direct solver, whereas a mean or slim structure gives an advantage to the direct solver

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In an objective of a continuation, one can in certain cases replace the base by the impression of fields MED. The "continuation" will begin then with the orders BEGINNING then LIRE_RESU.

6 Quality control

In a general way, the total quality of a study depends on several factors. Among the causes which can deteriorate the quality of a study, one can distinguish in particular:

- uncertainties on the data,
- choices of modeling (passage of the physique to digital),
- errors of discretization, once data established and modeling selected.

6.1 Uncertainties on the data

On this point uncertainties can be multiple because they can relate to each following aspect.

- The data material: once the law of behavior chosen, and its parameters correctly identified on adapted tests of characterization, it can remain an uncertainty on the values of the parameters of this law, which had with the variability of materials.
- The geometry exact of the structure to be modelled can comprise uncertainties: real dimensions are not those envisaged with the design, or the degradation of the shape of a part leads to a badly controlled geometry (apart from any aspect of discretization).
- Loadings (including thermics or due to other variables of orders: irradiation, hydration, drying, etc.) and the boundary conditions can present many uncertainties.
- Initial conditions, in particular those due to manufacturing (residual stress, initial work hardening).

For each dubious parameter evoked above, it will be sometimes necessary to carry out an analysis of sensitivity:

- that is to say the user carries out some simulations for extreme values of the dubious parameters, which is enough in the case of a monotonous variation to the result to these parameters (but it is not always the case: for example the dependence of the constraints to the extreme values of temperature, with coefficients material which are function, it is not commonplace.)
On this subject let us announce the possibility of carrying out very simply parametric calculations with *Code_Aster* (cf. [\[U2.08.07\] Distribution of parametric calculations](#))
- that is to say in the case of highly variable parameters, it carries out an analysis mechanic-reliability engineer, with OpenTurns (<http://www.openturns.org>) coupled to *Code_Aster*, in the platform Salomé-Meca [\[SV1.04.01\] Administrative of chained study Openturns/Aster](#)).

6.2 Choice of modeling and checking of the data

Even if the data are reliable, the quality of the results also depends on choices carried out by the user relating to simulation to carry out. The paragraphs precedent describe these choices. Let us point out some general advices:

- Beyond the grid, it can be useful to check the data of calculation, such as for example, to visualize the boundary conditions and loadings (direction and place of application), the assignments of materials, and the elementary characteristics (orientation of the beams, thicknesses, sections). For that, to use `IMPR_RESU/CONCEPT`.
- Other checks can be carried out directly in the command file; for example, to check the coherence of the system of units, the boundary conditions, the elementary characteristics, it is always useful to carry out a first elastic design, before any nonlinear study.
- To check the data material, it can be useful to carry out with the setting in data of *Code_Aster* a test simpler than the study, for example on material point (`SIMU_POINT_MAT`). Is the curve of traction and compression found?
- The calculation of the mass (or the volume) of the structure also is part of the simple but sometimes useful checks.

6.3 To control the errors due to the space discretization

On this point, we point out some general information here, but the reading of [\[U2.08.01\] Use of the indicators of error and associated strategies of adaptation of grids](#) more than is advised.

Independently of any desire to carry out adaptation of grid, we advise to check the initial grid with the order `MACR_INFO_MAIL` [\[U7.03.02\] Macro-order MACR_INFO_MAIL](#). This order makes it possible to realize, with few expenses, the following checks:

- to check the agreement of the grid with the initial geometry (in dimension, volume);
- to list them `GROUP_MA` and `GROUP_NO`, for a good modeling of the boundary conditions;
- to diagnose possible problems (connexity, holes, interpenetration of meshes);
- to provide quality standards of the meshes (evaluated mesh by mesh).

To more easily control the effect of the quality of the grid, an automatic strategy of adaptation of grid is operational: it is based on the software of adaptation of grid Lobster, which can be called directly since the command file of *Code_Aster* or in the platform Salomé-Meca, and uses either of the indicators of error allowing to control the adaptation, or the values of a field, or the jump of a field from one element to another. Several motivations appear to adapt a grid:

- The grid is very complicated to realize: one starts from a simple version and one entrusts to an automatic process the responsibility to refine it of.
- One wants to ensure itself convergence of the digital solution: rather than to realize with the hand of the increasingly fine grids, one lets the software seek itself the places where it would be necessary to refine the grid to increase the precision of the result.
- The conditions of calculation change during its unfolding: the zones which must be with a grid finely move. If one nets fine everywhere as of the beginning, the grid is too large. While adapting progressively, (refinement - déraffinement) the grid will be fine only at the places necessary: its size will be reduced and the quality of the solution will be good.

The zones to be refined can be located:

- Maybe with an indicator of error. Let us note that simplest (ZZ1, of Zhu-Zienkiewicz type) are very robust, available in 2D and 3D, and even if they do not provide best raising an error, their variations are enough to control the adaptation. The estimators in quantity of interest are more relevant to provide a terminal of the made mistake.
- Maybe with a field (deformation, variable interns) relevant. Attention, in plasticity, the constraint of Von Mises is not it always. One can use:
 - that is to say values extreme of this field (for example to ask to refine the 5% of elements which has the values strongest),
 - that is to say to control the adaptation by the jump of the values of this field to the border between two finite elements.
- Maybe by boxes (uniform refinement in geometrical zones).

For more information, to see [\[U2.08.01\] Use of the indicators of error and associated strategies of adaptation of grids](#)

6.4 Errors of discretization in time

For most nonlinearities (behavior, contact, great deformations) the temporal discretization influences the result. Results of convergence exist (extremely fortunately) in all the classical cases (élasto-visco-plasticity, contact), but it remains nevertheless to be made sure that for a step of selected time the solution is sufficiently close to the continuous solution in time.

The simplest solution is similar to uniform refinement for the adaptation of grid: it consists to uniformly refine the step of time on all the transient and to start again `STAT_NON_LINE`. This can be automated thanks to a functionality of `DEFI_LIST_INST` (see [\[U2.04.01\]](#) and [\[U4.34.03\]](#)).

Another criterion of control of the step of time is the subdivision according to a size of interest: `DEFI_LIST_INST/DELTA_Grandeur` redécouper indeed the step of time allows if the maximum variation of a given quantity (for example a component of plastic deformation) is higher than a provided threshold.

Moreover, for the elastoplastic behaviors, it is possible to consider directly the error due to the discretization in time, in a way similar to `RESI_RADI_RELA` (cf.3.2.4). If this criterion were not taken into account during calculation, it is possible to calculate it in postprocessing, in `CALC_CHAMP`: the component `ERR_RADI` option `DERA_ELGA` the estimate of error contains at every moment and in each point of integration.

7 References

- [1] "Mechanical of the structures", p.658, F.Voldoire; Y.Bamberger, Presses of the ENPC 2008.