Quasi-static nonlinear algorithm (STAT_NON_LINE)

Summary:

The operator STAT_NON_LINE [U4.51.03] of *Code_Aster* in the case of makes it possible a quasi-static request to integrate various types of non-linearities coming from the behavior of material, of great geometrical transformations or the conditions of contact/friction. One describes the total algorithm of resolution here employed.

The integration of the relations of behavior itself is described in the documents [R5.03….] and [R7.01….], (for example [R5.03.02] for elastoplasticity), to which one will be able to refer for more details.

For calculations in great geometrical transformations, one will be able to consult for example the document [R5.03.20] on nonlinear elasticity in great displacements, or the documents [R5.03.21], [R5.03.22] on the thermoelastoplasticity with isotropic work hardening.

For the contact friction, there exist three documents: [R5.03.50] on the discrete formulation of the contact/friction, [R5.03.52] for the hybrid formulation by elements of contact/friction, and [R5.03.53] on the contact in great slips with method XFEM.

For all that relates to piloting, it is necessary to refer to the document [R5.03.80].

1 Presentation

1.1 General information

STAT_NON_LINE is the operator of *Code_Aster* allowing to carry out nonlinear mechanical calculations when the effects of inertia are neglected (if one wants to take into account the effects of inertia, it is necessary to use DYNA_NON_LINE, to see [R5.05.05]).

Calculation relates a priori only to the mechanical variables (internal displacements, constraints, variables) by excluding any coupling with other physical phenomena (thermics,…). Consequently, the associated fields influencing the mechanical behavior (thermal, hydrous, metallurgical fields) are calculated as a preliminary by other operators (THER_LINEAIRE [U4.33.01], THER_NON_LINE [U4.33.02]), even by other codes (for example CODE_SATURNE for the mechanics of the fluids,…).

There is an exception with regard to the modeling thermo-hydro-mechanics (modeling known as 'THM') for which STAT_NON_LINE draft the whole of the coupled problem of the equations of diffusion of thermics, the pressure of (of) fluid (S) and of mechanical balance [R7.01.10].

It should be noted that when one speaks about moment of calculation in this document, one almost always refers to one pseudo-time, which does not have physical meaning and which is only used to parameterize the incremental algorithm. However, the moment keeps a physical significance in viscoplasticity and when the variables of order depend on it.

1.2 Types of nonlinearities

1.2.1 Nonlinear behaviors

The nonlinear relations of behavior are described in the documents [R5.03….], for the behavior generals, and [R7.01….] for géo-materials. The choice of the type of the behavior is done by the keyword factor BEHAVIOR . This led through the equilibrium equation to a nonlinear system which can be of two forms:

- The system depends explicitly on the field of displacements $\mathbf{u}$ compared to the configuration of reference, and parameterized by the moment of calculation (through inter alia the thermal evolution).
- The system depends implicitly on the field of displacements $\mathbf{u}$ by one ***implicit differential equation*** (for example elastoplasticity, the visco - plasticity, hypo-elasticity, etc). In this case, the relation of behavior is integrated as presented for example in [R5.03.02]: by connecting an increment of displacement $\Delta\mathbf{u}$ calculated starting from a mechanical state given (the mechanical state being represented by a field of displacements $\mathbf{u}$, a stress field σ and a field of internal variables α) with the stress field at the moment t calculation. The equilibrium equation thus leads to a nonlinear system in $\Delta\mathbf{u}$, but which is also parameterized by the moment of calculation through the facts of the case (variation of the mechanical loading and thermal evolution for example).

1.2.2 Great transformations

Whenever the assumption of the small disturbances (moderate displacements and deformations) is not checked, the method of resolution of the problem must then integrate the evolution of the geometry of the problem, handle a particular kinematics and use an adequate formulation of the law of behavior.

In practice, the assumption of the small deformations can be applied as long as the square of the modulus of deformation remains lower than the precision of calculations considered. In the same way, the assumption of small rotations can be applied as long as the product between the square of the swing angle and the modulus of deformation remains lower than the precision of calculations considered.

Various alternatives exist within *Code_Aster* ; our objective is not here to make a detailed presentation of it and we return to the various documents treating each problems specifically. It is appropriate to distinguish the formulations which operate on massive isoparametric elements (2D or 3D) and the formulations being used for

the elements of structure (beams, plates and hulls). For the cases of the massive isoparametric elements, one finds three great types of formulation of kinematics for the case of the great deformations:

- Kinematics DEFORMATION= 'PETIT_REAC' allows to treat an unspecified law of behavior in great deformations. The law is written in small deformations and the taking into account of the great deformations is done only by reactualizing the geometry. This formulation is not incrémentalement objective. Moreover, one can use it only if the behavior is isotropic, if the elastic strain are weak in front of the plastic deformations, if rotations remain weak (lower than $10°$) and if a sufficiently fine discretization in time is adopted. Moreover, the absence of the geometrical contribution in the tangent matrix can sometimes make convergence difficult (see [R5.03.21 for more details).
- Kinematics DEFORMATION= 'SIMO_MIEHE' allows to treat an elastoplastic law of behaviour with isotropic work hardening in great deformations, the law of ductile rupture known as “Rousselier” or the élasto (visco) plasticity with phase shift for the metallurgy (see [R5.03.21], [R5.03.06] and [R4.04.03]). This formulation is incrémentalement objective, without limitation on the level of the transformations applied but it is available only for the three quoted laws of behavior and allows to treat only the cases where the behavior is isotropic.
- Kinematics DEFORMATION= 'GDEF_LOG' also allows to treat any law of hypo-elastoplastic behavior. It is incrémentalement objective, without limitation on the level of the transformations applied and makes it possible to treat the case of the anisotropic behaviors (see [R5.03.24]).

To treat the great elastic strain, it is necessary to employ another formalism, called via DEFORMATION = 'GROT_GDEP' , which is usable for the relations of nonlinear behavior very-rubber bands in great displacements (see [R5.03.20] and [R5.03.22] for the case of the small deformations) or for the hyperelastic law of behavior (see [R5.03.19]).

Lastly, for the elements of structure (beam, plates or hulls), there exist specific formulations. One can quote:
- Beams in great displacements (see [R5.03.40]) or multifibre beams in great displacements (see [R3.08.09]). Keyword DEFORMATION=' GROT_GDEP'.
- Voluminal elements of hulls into nonlinear geometrical (see [R3.07.05]).

There do not exist elements of structures (beam, plate or hull) usable in great deformations in *Code_Aster*.

1.2.3 Unilateral contact and friction

For the contact and friction, one will refer to three documents: [R5.03.51] on the discrete contact with friction, [R5.03.52] for the hybrid formulation by elements of contact/friction and [R5.03.53] on the contact in great slips with method XFEM.

1.2.4 Limiting conditions and loadings

It is possible to define non-linear limiting conditions, i.e. depend on the displacement of the structure. There are two main categories of non-linear limiting conditions:
- For the loadings of Neumann, it is primarily the pressure: this one having to remain normal on the surface, the fact that the structure undergoes great transformations implies that the loading *depends* displacements. One will on this subject consult the documents [R3.03.07], [R3.03.04] and the §3.2 ;
- For the loadings of Dirichlet, Code_Aster allows for the moment only the loading of the type LIAISON_SOLIDE (see [U4.44.01]) which rigidifies in an exact way part of the structure. One will consult on this subject [R3.02.02];

In both cases, it is necessary to specify *explicitly* that this loading is non-linear (one speaks about loading ***follower***) thanks to keyword TYPE_CHARGE in word-key-factor EXCIT defining the loadings (see [U4.01.03]).

Note: in any general information, one can compare contact-friction to a mixed limiting condition (in displacement and pressure) which is non-linear.

1.3 Position of the nonlinear quasi-static problem

1.3.1 Problem general

As a consequence of paragraph 1.1, it is seen that it is legitimate to consider that the nonlinear problem has like unknown factor a displacement and that it is parameterized by time. Thus let us consider the quasi-static nonlinear problem by the classical expression of the principle of virtual work.

$$\mathbf{v}^T.\mathbf{L}^{\text{int}}(\mathbf{u},t)=\mathbf{v}^T.\mathbf{L}^{\text{ext}}(t) \qquad \forall \mathbf{v}=0 \tag{1}$$

where:

- t represent the variable of moment;
- $\mathbf{u}$ is the field of displacement taken starting from a configuration of reference;
- $\mathbf{v}$ is the field of virtual displacement kinematically acceptable;
- $\mathbf{L}^{\text{ext}}$ is the external mechanical loading to which the structure is subjected (pressure, imposed force, …) ;
- $\mathbf{L}^{\text{int}}$ represent the internal forces of the problem of quasi-static mechanics nonlinear. In the linear case, one has $\mathbf{L}^{\text{int}}(\mathbf{u},t)=\mathbf{K}.\mathbf{u}$, where $\mathbf{K}$ is the matrix of rigidity of the structure.

For the moment, one does not take account of the limiting conditions of Dirichlet. In fact, more precisely, $\mathbf{L}^{\text{int}}(\mathbf{u},t)$ is connected to the stress field $\boldsymbol{\sigma}$ by the operator of the work of the virtual deformations $\mathbf{Q}^T$ according to the following relation:

$$\mathbf{L}^{\text{int}}(\mathbf{u},t)=\mathbf{Q}^T(\mathbf{u}).\boldsymbol{\sigma} \tag{2}$$

In small displacements, $\mathbf{Q}^T$ is independent of displacements; for great displacements, it is not any more the case. One gives oneself a discretization of the time interval to be calculated:

$$t\rightarrow\left[t_0,\cdots,t_i,\cdots,t_n\right] \tag{3}$$

The stress field $\boldsymbol{\sigma}_i$ at the moment t_i is written $\boldsymbol{\sigma}(\mathbf{u}_i,\beta_i,t_i,\mathbf{H}_{i-1})$, if one notes β_i fields of variables of order and $\mathbf{H}_{i-1}$ last history of the structure. For the elastic behaviors, the history does not intervene: the unit $\mathbf{H}_{i-1}$ is thus empty. For the incrémentaux behaviors, the history is the whole of the states (fields of displacements, constraints and variables internal) at the previous moment: $\mathbf{H}_{i-1}=\left\{\mathbf{u}_{i-1},\boldsymbol{\sigma}_{i-1},\boldsymbol{\alpha}_{i-1},t_{i-1}\right\}$.

In the case general, the dependence of the operator $\mathbf{L}^{\text{int}}$ is, as we saw in [the §1.1], implicit compared to time: it results from the integration of the relation of behavior in time (for the problems of elastoplasticity for example). The explicit dependence compared to time in particular in the case of appears relations of take behavior into account a phenomenon of work hardening by time (time-hardening) or in the case of ageing.

The formulation of the quasi-static problem consists in expressing the balance of the structure (the internal forces are equal to the external forces) for a continuation of moments of calculation $\left(t_i\right)_{1\leq i\leq I}$ who parameterize the loading, one will note the quantities at the moment t_i by the index i (for example $\mathbf{L}^{\text{int}}(\mathbf{u_i},t_i)=\mathbf{L}_i^{\text{int}}$):

$$\mathbf{L}_i^{\text{int}}=\mathbf{L}_i^{\text{ext}} \tag{4}$$

What amounts cancelling in $(\mathbf{u}_i,t_i)$ the vector $\mathbf{R}_i(\mathbf{u}_i,t_i)$ known as vector residue of balance, defined by:

$$\mathbf{R}_i(\mathbf{u}_i,t_i)=\mathbf{L}_i^{\text{int}}-\mathbf{L}_i^{\text{ext}} \tag{5}$$

The state of the structure in t_0 is supposed to be known. One carries out I increments (or not) of load. The unknown factors are calculated in an incremental way by the total algorithm of resolution (even for the elastic behaviors). From $\mathbf{u}_{i-1}$, solution satisfying balance in t_{i-1}, one determines $\Delta\mathbf{u}_i$ who will allow to obtain the solution in t_i :

$$\begin{cases} t_i=t_{i-1}+\Delta t_i \\ \mathbf{u}_i=\mathbf{u}_{i-1}+\Delta\mathbf{u}_i \end{cases} \tag{6}$$

The increment $\Delta\mathbf{u}_i$ is initially estimated by linearizing the problem compared to time around $(\mathbf{u}_{i-1},t_{i-1})$ (phase known as of prediction or Euler). Then one uses a method of Newton or one of his alternatives to solve

the equation (4) in an iterative way (a continuation is calculated $\Delta \mathbf{u}_i^n$ where the exhibitor n is the number of the iteration). Besides these variables, for the incremental relations of behavior, one needs to know in t_{i-1} the stress field $\boldsymbol{\sigma}_{i-1}$ and the field of internal variables $\boldsymbol{\alpha}_{i-1}$ (see [R5.03.02] for an example).

1.3.2 Limiting conditions of Dirichlet

We imposed that the field of virtual displacements is *kinematically* acceptable, i.e. he observes the boundary conditions in displacements (or conditions of Dirichlet). In general manner, Lbe conditions of Dirichlet ***linear*** are written :

$$\sum_{j=1}^{r} \alpha_j u_j = \beta(t) \tag{7}$$

With u_j the list of r Degrés of freedom, α_j coefficients and β the second member who can depend on time.

In Code_Aster, there are two manners of taking into account these conditions:

- By a method known as “kinematic” (definition by AFFE_CHAR_CINE) who uses a method of pseudonym elimination in the resulting linear system (see [U4.44.03]). In this case, one can define only simple limiting conditions such as $r=1$;
- By a method of dualisation (definition by AFFE_CHAR_MECA) who uses the technique of the Lagrange doubles (see [R3.01.01]).

It is possible to eliminate from the limiting conditions dualized by the use of a special method which one describes in [R3.03.05], but only by using the solvor PETSc.

We now describe the manner of taking into account the limiting conditions ***dualized*** in the resolution of a non-linear problem. Initially, we will suppose that limiting conditions (7) can be written in the following discrete form:

$$\mathbf{B}.\mathbf{u} = \mathbf{u}^d(t) \tag{8}$$

$\mathbf{B}$ is an operator *linear* space of the fields of displacements on a space of functions defined on part of the edge of the structure, $\mathbf{u}^d$ is a function given on this part. The dualisation of the boundary conditions of Dirichlet $\mathbf{B}.\mathbf{u} = \mathbf{u}^d(t)$ conduit to be modified (4) in the following way:

$$\begin{cases} \mathbf{L}^{\text{int}}(\mathbf{u},t) + \mathbf{B}^T.\boldsymbol{\lambda} = \mathbf{L}^{\text{ext}}(t) \\ \mathbf{B}.\mathbf{u} = \mathbf{u}^d(t) \end{cases} \tag{9}$$

The unknown factors are now, at any moment t, the couple $(\mathbf{u},\boldsymbol{\lambda})$, where $\boldsymbol{\lambda}$ represent them *multipliers of Lagrange* boundary conditions of Dirichlet. The vector $\mathbf{B}^{\mathbf{T}}.\lambda$ be interpreted then like the opposite of the reactions of support to the corresponding nodes.
By noting the quantities at the moment t_i by the index i :

$$\begin{cases} \mathbf{L}_i^{\text{int}} + \mathbf{B}^T.\boldsymbol{\lambda}_i = \mathbf{L}_i^{\text{ext}} \\ \mathbf{B}.\mathbf{u}_i = \mathbf{u}_i^d \end{cases} \tag{10}$$

The vector residue of balance $\mathbf{R}_i(\mathbf{u}_i,\boldsymbol{\lambda}_i,t_i)$ is worth now:

$$\mathbf{R}_i(\mathbf{u}_i,\boldsymbol{\lambda}_i,t_i) = \begin{pmatrix} \mathbf{L}_i^{\text{int}} + \mathbf{B}^{\mathbf{T}}.\boldsymbol{\lambda}_i - \mathbf{L}_i^{\text{ext}} \\ \mathbf{B}.\mathbf{u}_i - \mathbf{u}_i^d \end{pmatrix} \tag{11}$$

The unknown factors are always calculated in an incremental way by the total algorithm of resolution. From $(\mathbf{u}_{i-1},\boldsymbol{\lambda}_{i-1})$, solution satisfying balance in t_{i-1}, one determines $\Delta\mathbf{u}_i$ and $\Delta\boldsymbol{\lambda}_i$ who will allow to obtain the solution in t_i :

$$\begin{cases} t_i = t_{i-1} + \Delta t_i \\ \mathbf{u}_i = \mathbf{u}_{i-1} + \Delta \mathbf{u}_i \\ \boldsymbol{\lambda}_i = \boldsymbol{\lambda}_{i-1} + \Delta \boldsymbol{\lambda}_i \end{cases} \quad (12)$$

2 Method of Newton

2.1 Principle of the method

The method of Newton is a classical method of resolution of the equations of the type searches of zero. Let us consider a vector function $\mathbf{F}$ non-linear of the vector $\mathbf{x}$. One seeks the zero of this function, i.e.:

$$\mathbf{F}(\mathbf{x})=0 \tag{13}$$

The method of Newton consists in building a vector series $\mathbf{x}^n$ converging towards the solution $\mathbf{x}$. To find the new one reiterated $\mathbf{x}^{n+1}$, one approaches $\mathbf{F}(\mathbf{x}^{n+1})$ by a development limited to the order one around $\mathbf{x}^n$ and one expresses that $\mathbf{F}(\mathbf{x}^{n+1})$ must be null:

$$0=\mathbf{F}(\mathbf{x}^{n+1})\approx\mathbf{F}(\mathbf{x}^n)+\mathbf{F}'(\mathbf{x}^n)(\mathbf{x}^{n+1}-\mathbf{x}^n) \tag{14}$$

That is to say still:

$$\mathbf{F}'(\mathbf{x}^n)(\mathbf{x}^{n+1}-\mathbf{x}^n)=-\mathbf{F}(\mathbf{x}^n) \tag{15}$$

Finally:

$$\mathbf{x}^{n+1}=\mathbf{x}^n-\left[\mathbf{F}'(\mathbf{x}^n)\right]^{-1}.\mathbf{F}(\mathbf{x}^n) \tag{16}$$

$\mathbf{F}'(\mathbf{x})$ is the tangent linear application associated with the function $\mathbf{F}$. The derivative at the point $\mathbf{x}$ in the direction $\mathbf{h}$ is defined like the following directional derivative:

$$\mathbf{F}'(\mathbf{x}).\mathbf{h}=\lim_{\theta\to 0}\frac{\mathbf{F}(\mathbf{x}+\theta.\mathbf{h})-\mathbf{F}(\mathbf{x})}{\theta} \tag{17}$$

The matrix of $\mathbf{F}'(\mathbf{x})$ in the bases chosen for the vector spaces concerned is called the matrix *jacobienne* of $\mathbf{F}$ at the point $\mathbf{x}$. When $\mathbf{F}$ is a function of an Euclidean vector space with actual values, $\mathbf{F}'(\mathbf{x})$ is a linear form, and one can show that there exists a vector (single), noted $\nabla\mathbf{F}(\mathbf{x})$ and called the gradient of $\mathbf{F}$, such as:

$$\mathbf{F}'(\mathbf{x}).\mathbf{h}=\mathbf{h}^T.\nabla\mathbf{F}(\mathbf{x}) \tag{18}$$

I.e. the scalar product of $\mathbf{h}$ and of the gradient of $\mathbf{F}$.

When one is close to the solution, the convergence of the method of Newton is quadratic i.e. the number of zeros after the comma in the error doubles with each iteration (0.19 – 0.036 – 0.0013 – 0.0000017 for example). But this method (using the true tangent) has several disadvantages:

- It requires the calculation of the tangent to each iteration, which is all the more expensive as size of problem is large (especially if a direct solvor is used),
- If the increment is large, the tangent (known as coherent or consistent) can lead to divergences of the algorithm,
- It can not be symmetrical, which obliges to use particular solveurs.

For this reason one can use other matrices instead of the tangent matrix: the elastic matrix, a tangent matrix obtained before, the symmetrized tangent matrix,…

2.2 Adaptation of the method of Newton to the posed problem

Initially, one does not take into account the boundary conditions of Dirichlet. One must solve a system (non-linear because dependent on $\mathbf{u}_i$) form:

$$\mathbf{L}_i^{\text{int}}(\mathbf{u}_i)=\mathbf{L}_i^{\text{méca}}(\mathbf{u}_i) \tag{19}$$

where $\mathbf{L}_i^{\text{méca}}$ will indicate from now on, at the moment t_i, the part *mechanics* total external loading $\mathbf{L}_i^{\text{ext}}$ in order to distinguish it from the thermal loading. Let us note that the mechanical loading $\mathbf{L}_i^{\text{méca}}(\mathbf{u}_i)$ can depend on displacements $\mathbf{u}_i$ in the case of forces known as "following" like the pressure or the centrifugal force (see [§3.2]). By using the notations of [the §2.1], that amounts cancelling the vector function $\mathbf{R}$ defined by:

$$\mathbf{R}(\mathbf{u}_i, t_i) = \mathbf{L}_i^{\text{int}} - \mathbf{L}_i^{\text{méca}} \tag{20}$$

Internal forces $\mathbf{L}_i^{\text{int}}$ can ***symbolically*** to be noted $\mathbf{Q}_i^T.\boldsymbol{\sigma}_i$, where $\mathbf{Q}_i^T$ is the matrix associated with the operator divergence (expression of the agricultural work of virtual deformations). Lbe internal forces express themselves then:

$$\mathbf{L}_i^{\text{int}} = \mathbf{Q}_i^T.\boldsymbol{\sigma}_i = \int_\Omega \boldsymbol{\varepsilon}(\mathbf{w}_i) : \boldsymbol{\sigma}(\mathbf{u}_i).d\Omega \tag{21}$$

And forces of the mechanical loading:

$$\mathbf{L}_i^{\text{méca}} = \int_\Omega \mathbf{f}_i.\mathbf{w}_i.d\Omega + \int_\Gamma \mathbf{t}_i.\mathbf{w}_i.d\Gamma \tag{22}$$

Where:

- $\mathbf{w}_i$ indicate the field of virtual displacements;
- $\mathbf{f}_i$ désignE voluminal forces applying to the moment t_i on Ω ;
- $\mathbf{t}_i$ désig surface forces applying to the moment t_i on the border Γ of Ω .

The application of the method of Newton results in solving a linear succession of problems of the type (n is the number of the iteration of Newton, i that of the variable of moment):

$$\mathbf{K}_i^n.\Delta\mathbf{u}_i^{n+1} = \mathbf{L}_i^{\text{méca},n} - \mathbf{L}_i^{\text{int},n} \tag{23}$$

One notes $\delta\mathbf{u}_i^{n+1} = \mathbf{u}_i^{n+1} - \mathbf{u}_i^n$ the increment of displacement between two successive iterations of Newton. The matrix $\mathbf{K}_i^n$ is the matrix of tangent rigidity in $\mathbf{u}_i^n$ and the vector $\mathbf{L}_i^{\text{int},n}$ represent the internal forces with $n^{\text{ième}}$ iteration of Newton of $i^{\text{ème}}$ pas de charges. Quantity $\mathbf{R}_i^n = \left(\mathbf{L}_i^{\text{méca},n} - \mathbf{L}_i^{\text{int},n}\right)$ represent the not balanced forces, which one calls the "residue of balance". The matrix $\mathbf{K}_i^n$ is the matrix of the tangent linear application of the function $\mathbf{R}_i^n$, it is thus worth:

$$\mathbf{K}_i^n = \left.\frac{\partial\mathbf{R}_i^n}{\partial\mathbf{u}}\right|_{(\mathbf{u}_i^n, t_i)} = \left.\frac{\partial\mathbf{L}_i^{\text{int},n}}{\partial\mathbf{u}}\right|_{(\mathbf{u}_i^n, t_i)} - \left.\frac{\partial\mathbf{L}_i^{\text{méca},n}}{\partial\mathbf{u}}\right|_{(\mathbf{u}_i^n, t_i)} \tag{24}$$

In the absence of following forces [§3.2], the second term is null. It thus does not remain of the matrix $\mathbf{K}_i^n$ that the derivative at the point $\mathbf{u}_i^n$ internal forces compared to displacements:

$$\mathbf{K}_i^n = \left.\frac{\partial\mathbf{L}_i^{\text{int},n}}{\partial\mathbf{u}}\right|_{(\mathbf{u}_i^n, t_i)} \tag{25}$$

A small error in the evaluation of the internal forces can have serious consequences, because it is their exact calculation which guarantees, if one converges, that it will be towards the sought solution. On the other hand, it is not always necessary to use the true tangent matrix, whose calculation and factorization are expensive. For example, an alternative of the method uses the elastic matrix $\mathbf{K}_{\text{élas}}$. Method using the true tangent matrix $\mathbf{K}_i^n$ (known as also coherent or consistent matrix) is called the method of Newton; methods using of other matrices (such as for example the elastic matrix $\mathbf{K}_{\text{élas}}$) are called methods of Newton modified or methods of quasi-Newton. The choice between a tangent matrix (the last obtained or a preceding matrix) and an elastic matrix is carried out in *Code_Aster* via the keyword 'TANGENT' MATRICE= or MATRICE=' ELASTIQUE' keyword factor NEWTON. Moreover, it is possible to use a matrix of discharge, i.e. of a matrix with constant internal variables (the evolution of nonthe linearities is thus not taken into account in this matrix), below a certain step of time, for certain laws of behavior. One will refer to documentation [U4.51.03] for the use of this functionality.

The method of Newton with consistent tangent matrix can be illustrated simply using the diagram of [Figure 2.2.1-a].

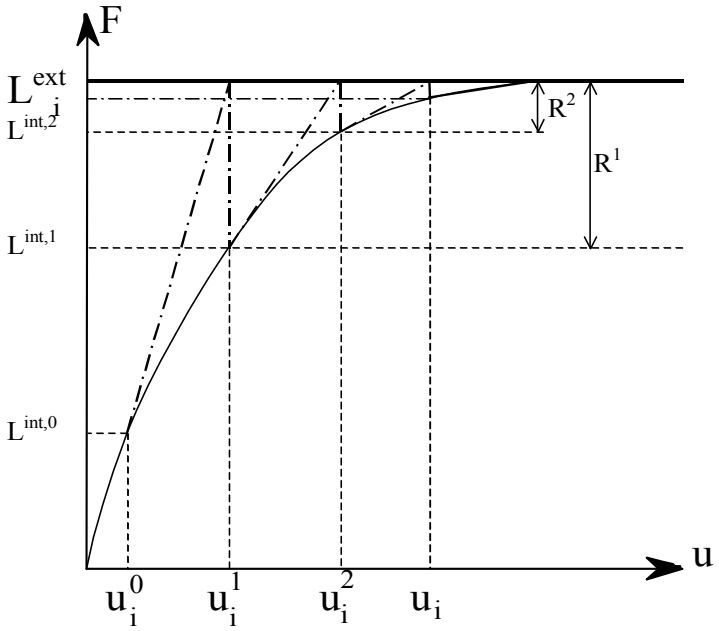

Figure 2.2.1-a

One connects with the loop of the iterations of Newton which makes it possible, with convergence, to obtain the values of $\Delta \mathbf{u}_i$, and thus those of $\mathbf{u}_i$ by application of the equation (6):

$$\mathbf{u}_i = \mathbf{u}_{i-1} + \Delta \mathbf{u}_i \tag{26}$$

2.3 Phase of prediction of Euler

The experiment shows that the convergence of the method of Newton is strongly dependent on a wise choice of the initial estimate: “more the initial estimate is close to the solution, plus the algorithm converges quickly”. To start the iterative process of the method, it is thus useful to determine “a good” initial increment $\Delta \mathbf{u}_i^0$. For that, one linearizes compared to time the continuous problem: it is what is called the phase of *prediction*.

2.3.1 Linearization

One will thus linearize the system (19) compared to time around $\mathbf{u}_{i-1}$. One starts by linearizing the internal forces $\mathbf{L}_i^{\text{int}}$:

$$\mathbf{L}_i^{\text{int}} \approx \mathbf{L}_{i-1}^{\text{int}} + \left.\frac{\partial \mathbf{L}^{\text{int}}}{\partial \mathbf{u}}\right|_{\mathbf{u}_{i-1}} . \Delta \mathbf{u}_i^0 + \left.\frac{\delta \mathbf{L}^{\text{int}}}{\delta t}\right|_{t_{i-1}} \tag{27}$$

It is supposed that the mechanical loading does not depend on time (the following loads are excluded), therefore:

$$\begin{cases} \mathbf{L}_i^{\text{méca}} = \mathbf{L}_{i-1}^{\text{méca}} + \Delta \mathbf{L}_i^{\text{méca}} \\ \mathbf{u}_i^d = \mathbf{u}_{i-1}^d + \Delta \mathbf{u}_i^d \end{cases} \tag{28}$$

While reinjecting 27and 28 in the first equation of the system 26, one obtains for the equilibrium equation:

$$\mathbf{L}_{i-1}^{\text{int}} + \left.\frac{\partial \mathbf{L}^{\text{int}}}{\partial \mathbf{u}}\right|_{\mathbf{u}_{i-1}} . \Delta \mathbf{u}_i^0 + \left.\frac{\delta \mathbf{L}^{\text{int}}}{\delta t}\right|_{t_{i-1}} . \Delta t_i = \mathbf{L}_{i-1}^{\text{méca}} + \Delta \mathbf{L}_i^{\text{méca}} \tag{29}$$

There is balance at the moment t_{i-1} , i.e.:

$$\mathbf{L}_{i-1}^{\text{int}} = \mathbf{L}_{i-1}^{\text{méca}} \tag{30}$$

And it thus remains:

$$\left.\frac{\partial \mathbf{L}^{\text{int}}}{\partial \mathbf{u}}\right|_{\mathbf{u}_{i-1}} . \Delta \mathbf{u}_i^0 + \left.\frac{\delta \mathbf{L}^{\text{int}}}{\delta t}\right|_{t_{i-1}} . \Delta t_i = \Delta \mathbf{L}_i^{\text{méca}} \tag{31}$$

One obtains the system of equations allowing to calculate predictive values $\Delta \mathbf{u}_i^0$:

$$\left.\frac{\partial \mathbf{L}^{\text{int}}}{\partial \mathbf{u}}\right|_{\mathbf{u}_{i-1}} . \Delta \mathbf{u}_i^0 = \Delta \mathbf{L}_i^{\text{méca}} - \left.\frac{\delta \mathbf{L}^{\text{int}}}{\delta t}\right|_{t_{i-1}} . \Delta t_i \tag{32}$$

2.3.2 Tangent matrix of prediction

Quantity $\left.\frac{\partial \mathbf{L}^{\text{int}}}{\partial \mathbf{u}}\right|_{\mathbf{u}_{i-1}}$ indicate the partial derivative with time constant of $\mathbf{L}_{i-1}^{\text{int}}$, it can develop:

$$\mathbf{K}_{i-1} = \left.\frac{\partial \mathbf{L}^{\text{int}}}{\partial \mathbf{u}}\right|_{\mathbf{u}_{i-1}} = \left(\mathbf{Q}_{i-1}^T . \left.\frac{\partial \boldsymbol{\sigma}}{\partial \mathbf{u}}\right|_{\mathbf{u}_{i-1}} + \left.\frac{\partial \mathbf{Q}^T}{\partial \mathbf{u}}\right|_{\mathbf{u}_{i-1}} . \boldsymbol{\sigma}_{i-1} \right) \tag{33}$$

The matrix $\mathbf{K}_{i-1}$ tangent matrix of prediction is called. Dependence of the matrix $\mathbf{Q}$ compared to displacements is neglected on the assumption of small displacements: the term $\left.\frac{\partial \mathbf{Q}^T}{\partial \mathbf{u}}\right|_{\mathbf{u}_{i-1}}$, known as term of geometrical rigidity, thus disappears from 33. This term is taken into account for the great transformations (see §1.2.2). For the developers, let us specify that the calculation of the tangent matrix at the time of the phase of prediction is carried out via the option of calculation `RIGI_MECA_TANG`.

2.3.3 Alternatives of the prediction

There exist other options of prediction available in `STAT_NON_LINE`.

- One can use an elastic matrix $\mathbf{K}_{\text{élas}}$ instead of the tangent matrix of speed $\mathbf{K}_{i-1}$, it is the option `PREDICTION=' ELASTIQUE'` (option `RIGI_MECA`).
- One can use a secant matrix $\mathbf{K}_{\text{sécante}}$ instead of the tangent matrix of speed $\mathbf{K}_{i-1}$, it is the option `PREDICTION=' SECANTE'` (option `RIGI_MECA_ELAS`). The secant matrix is an elastic matrix whose Young modulus is used by applying the damage (see for example [R5.03.18] for more details)
- One can use an increment of displacement previously calculated instead of the estimate, it is the option `PREDICTION=' DEPL_CALCULE'`. In this case one makes no inversion of system and it $\Delta \mathbf{u}_i^0$ is directly given. See documentation [U4.51.03] for its use.
- One can use an increment of displacement extrapolated compared to the preceding step. One calculates the estimate of the increment of displacement starting from the total increment obtained as solution with the step of previous time (balanced by the report of the steps of time). It is the option `PREDICTION=' EXTRAPOL'`.

In these the last two cases, in order to ensure that initial displacement is kinematically acceptable, one projects the estimate on the whole of the fields kinematically acceptable (i.e satisfying the boundary conditions with Dirichlet) according to the standard given by the matrix ***rubber band*** , which must thus be calculated.

2.3.4 Vector second member of the variables of order

A variable of order $\beta(t)$ is a scalar quantity, function of time and space[1], data a priori by the user via the keyword `AFFE_VARC` in the operator `AFFE_MATERIAU`. It is one *parameter* problem and not one *unknown factor*. Quantity $\left.\frac{\delta \mathbf{L}^{\text{int}}}{\delta t}\right|_{t_{i-1}}$ indicate the partial differential, compared to t and with $\mathbf{u}$ constant, of

1 To be more precise, a variable of order is assigned to a mesh. It thus is not about a function of the geometry (and thus of displacements), but of the topology of the grid.

$\mathbf{L}^{\text{int}}=\mathbf{Q}.\boldsymbol{\sigma}(t,\beta(t))$. The purpose of this particular notation is to draw attention to the fact that for n_{varc} variables of orders, the total differential is written:

$$\frac{\delta\boldsymbol{\sigma}}{\delta t}=\frac{\partial\boldsymbol{\sigma}}{\partial t}+\sum_{j=1,n_{varc}}\frac{\delta\boldsymbol{\sigma}}{\delta\beta^{j}}.\frac{\delta\beta^{j}}{\delta t} \tag{34}$$

If one takes as example the variable of order describing the temperature θ :

$$\frac{\delta\boldsymbol{\sigma}}{\delta t}=\frac{\partial\boldsymbol{\sigma}}{\partial t}+\frac{\delta\boldsymbol{\sigma}}{\delta\theta}.\frac{\delta\theta}{\delta t} \tag{35}$$

It is supposed that the temperature varies linearly between the two moments:

$$\frac{\delta\theta}{\delta t}=\frac{\Delta\theta_i}{\Delta t_i} \tag{36}$$

Dependence of $\boldsymbol{\sigma}$ compared to time and compared to the temperature allows to write:

$$\left.\frac{\delta\mathbf{L}^{int}}{\delta t}\right|_{t_{i-1}}=\frac{\delta}{\delta t}\left(\mathbf{Q}_{i-1}^{T}.\boldsymbol{\sigma}_{i-1}\right)=\mathbf{Q}_{i-1}^{T}.\left(\left.\frac{\partial\boldsymbol{\sigma}}{\partial t}\right|_{t_{i-1}}+\left.\frac{\partial\boldsymbol{\sigma}}{\partial\theta}\right|_{t_{i-1}}.\frac{\Delta\theta_i}{\Delta t_i}\right) \tag{37}$$

Because $\mathbf{Q}$ does not depend on time and thus $\frac{\delta}{\delta t}\left(\mathbf{Q}^{T}\right)=0$. The vector $\Delta\mathbf{L}_i^{\text{varc}}$, of which the expression is given by 38, is the increment of loading of temperature (attention to the change of sign!) which one generalized with all them *variables of orders* : metallurgical temperature, irradiation, phases (see *[R4.04.02]),*…

$$\Delta\mathbf{L}_i^{varc}=-\left.\frac{\delta\mathbf{L}^{int}}{\delta t}\right|_{t_{i-1}}.\Delta t_i=-\mathbf{Q}_{i-1}^{T}.\left(\left.\frac{\partial\boldsymbol{\sigma}}{\partial t}\right|_{t_{i-1}}.\Delta t_i+\sum_{j=1,n_{varc}}\left(\left.\frac{\partial\boldsymbol{\sigma}}{\partial\beta^{j}}\right|_{t_{i-1}}.\Delta\beta_i^{j}\right)\right) \tag{38}$$

One currently does not take account of the explicit dependence of the constraints compared to time and thus the first term of 38 zero are worth. And thus finally:

$$\Delta\mathbf{L}_i^{varc}=-\mathbf{Q}_{i-1}^{T}.\left(\sum_{j=1,n_{varc}}\left(\left.\frac{\partial\boldsymbol{\sigma}}{\partial\beta^{j}}\right|_{t_{i-1}}.\Delta\beta_i^{j}\right)\right) \tag{39}$$

The increment of loading *variables of order* $\Delta\mathbf{L}_i^{\text{varc}}$, resulting from the derivation of the internal forces compared to the variables of order is an estimate of the effect of a variation of the variables of orders.

In the case of the temperature, if one notes K the hydrostatic module of compression and α the thermal dilation coefficient, the thermal stress is written:

$$\boldsymbol{\sigma}_i^{\text{ther}}=-3.K.\alpha.\Delta\theta_i.\mathbf{I}+\boldsymbol{\sigma}_{i-1}^{\text{ther}}\quad\text{if}\quad\Delta\theta_i=\theta_i-\theta_{i-1} \tag{40}$$

Where $\mathbf{I}$ is the matrix identity. And thus, while applying 39:

$$\Delta\mathbf{L}_i^{ther}=-\left(\mathbf{Q}_{i-1}^{T}.\left.\frac{\partial\boldsymbol{\sigma}}{\partial\theta}\right|_{t_{i-1}}\right).\Delta\theta_i=3.K.\alpha.\Delta\theta_i.\left(\mathbf{Q}_{i-1}^{T}.\mathbf{I}\right) \tag{41}$$

In the elastic case, they are the internal forces associated with a thermal dilation (it is not strictly speaking a loading, that is assimilated rather to the effect of an initial deformation). This estimate is used in the phase of prediction and the criterion of stop. If thermal dilations make leave the structure of the elastic range (plasticity for example), this estimate will be corrected at the time of the iterations of Newton.

2.3.5 Vector second member of the mechanical loading

The increment of loading *mechanics* $\Delta\mathbf{L}_i^{\text{méca}}$ is composed of the dead loads (independent of the geometry, like gravity) and of the following loads. Actually, there exist cases (the first increment of load, for example) where $\mathbf{L}_{i-1}^{\text{méca}}$ is unknown. It is pointed out that the increment of loading (28) is written:

$$\mathbf{L}_i^{\text{méca}} = \mathbf{L}_{i-1}^{\text{méca}} + \Delta \mathbf{L}_i^{\text{méca}} \tag{42}$$

There is balance at the moment t_{i-1} , therefore while applying 30:

$$\Delta \mathbf{L}_i^{\text{méca}} = \mathbf{L}_i^{\text{méca}} - \mathbf{L}_{i-1}^{\text{int}} \tag{43}$$

The expression of the internal forces to the step of previous time $\mathbf{L}_{i-1}^{\text{int}}$ imply either to save this vector of preceding calculation if there exists (taken again of a former calculation), or to integrate the law of behavior starting from the initial state given by the user (what can be expensive). By preoccupation of simplicity and an effectiveness, one chooses not to reinstate the law of behavior and one expresses simply the internal forces like the nodal forces by taking the constraints known at this moment, that is to say:

$$\mathbf{L}_{i-1}^{int} = \mathbf{Q}_{i-1}^{T} . \boldsymbol{\sigma}_{i-1} \tag{44}$$

From where the new expression:

$$\Delta \mathbf{L}_i^{\text{méca}} = \mathbf{L}_i^{\text{méca}} - \mathbf{Q}_{i-1}^{T} . \boldsymbol{\sigma}_{i-1} \tag{45}$$

Direct calculation from (44) request with the user to take care of coherence enters the field of the constraints, the fields of displacements and internal variables (DEPL , SIGM and VARI in ETAT_INIT). with respect to the integration of the law of behavior in the case of a resumption of calculation.

2.3.6 Linear system

By reinjecting the expression of $\left.\frac{\partial \mathbf{L}^{\text{int}}}{\partial \mathbf{u}}\right|_{\mathbf{u}_{i-1}}$ (equation 33) , of $\left.\frac{\delta \mathbf{L}^{\text{int}}}{\delta t}\right|_{t_{i-1}}$ (equation 38) and $\Delta \mathbf{L}_i^{\text{méca}}$ (equation 45) in 32, the system of equations in prediction is written:

$$\mathbf{K}_{i-1} . \Delta \mathbf{u}_i^0 = \mathbf{L}_i^{\text{méca}} - \mathbf{Q}_{i-1}^{T} . \boldsymbol{\sigma}_{i-1} + \Delta \mathbf{L}_i^{\text{varc}} \tag{46}$$

2.4 Phase of correction of Newton

At the conclusion of the phase of prediction, we find ourselves with an estimate of the increment of displacements $\Delta \mathbf{u}_i^0$. If this estimate is exact (modulo the application of the convergence criteria described to the §2.5), then the solution is obtained ***converged*** for the step of time t_i :

$$\mathbf{u}_i^{\text{convergé}} = \mathbf{u}_{i-1} + \Delta \mathbf{u}_i^0 \tag{47}$$

But if it is not the case, one must find the value $\Delta \mathbf{u}_i$ increment of displacement starting from the value $\mathbf{u}_{i-1}$ obtained with preceding balance (urgent t_{i-1}):

$$\mathbf{u}_i^{\text{convergé}} = \mathbf{u}_{i-1} + \Delta \mathbf{u}_i \tag{48}$$

If the phase of prediction converged, one thus has crudely:

$$\Delta \mathbf{u}_i = \Delta \mathbf{u}_i^0 \tag{49}$$

If not, one takes as initial value $\Delta \mathbf{u}_i^0$ obtained at the conclusion of the phase of prediction, before correcting by the iterations $\delta \mathbf{u}_i^n$ method of Newton. With a number n_{CV} sufficient of iterations of Newton (always with the arbitration of the convergence criteria):

$$\mathbf{u}_i^{\text{convergé}} = \mathbf{u}_{i-1} + \Delta \mathbf{u}_i^0 + \sum_{j=1}^{n=n_{CV}} \delta \mathbf{u}_i^j \tag{50}$$

As long as one did not converge (if the iteration count of Newton is not sufficient), one notes:

$$\Delta \mathbf{u}_i^n = \Delta \mathbf{u}_i^0 + \sum_{j=1}^{n<n_{CV}} \delta \mathbf{u}_i^j \tag{51}$$

Total displacement, for the step of time i and the iteration of Newton n will thus be written:

$$\mathbf{u}_i^n = \mathbf{u}_{i-1} + \Delta \mathbf{u}_i^n \tag{52}$$

With each iteration, one must solve a system allowing to determine $\delta \mathbf{u}_i^n$, increments of displacements since the result $\mathbf{u}_i^{n-1}$ preceding iteration:

$$\mathbf{u}_i^{n-1} = \mathbf{u}_{i-1} + \mathbf{u}_i^0 + \sum_{j=1}^{n-1} \delta \mathbf{u}_i^j \tag{53}$$

One also notes:

$$\Delta \mathbf{u}_i^{n-1} = \Delta \mathbf{u}_i^0 + \sum_{j=1}^{n-1} \delta \mathbf{u}_i^j \tag{54}$$

That is to say still:

$$\mathbf{u}_i^n = \mathbf{u}_i^{n-1} + \delta \mathbf{u}_i^n = \mathbf{u}_{i-1} + \Delta \mathbf{u}_i^{n-1} + \delta \mathbf{u}_i^n \tag{55}$$

2.4.1 Linearization

One must linearize the system (19) compared to the unknown factors in $\mathbf{u}_i^n$ with t_i constant. One starts by linearizing the internal forces $\mathbf{L}_i^{\text{int},n}$:

$$\mathbf{L}_i^{\text{int},n} \approx \mathbf{L}_i^{\text{int},n-1} + \left.\frac{\partial \mathbf{L}^{\text{int}}}{\partial \mathbf{u}}\right|_{\mathbf{u}_i^{n-1}} . \delta \mathbf{u}_i^n \tag{56}$$

It is supposed that the mechanical loading does not depend on time (the following loads are excluded).

2.4.2 Linear system

While reinjecting (56) in the equation (19), one obtains for the equilibrium equation:

$$\mathbf{L}_i^{\text{int},n-1} + \left.\frac{\partial \mathbf{L}^{\text{int}}}{\partial \mathbf{u}}\right|_{\mathbf{u}_i^{n-1}} . \delta \mathbf{u}_i^n = \mathbf{L}_i^{\text{méca}} \tag{57}$$

Quantity $\left.\frac{\partial \mathbf{L}^{\text{int}}}{\partial \mathbf{u}}\right|_{\mathbf{u}_i^{n-1}}$ is called coherent tangent matrix and it is noted $\mathbf{K}_i^{n-1}$:

$$\mathbf{K}_i^{n-1} = \left.\frac{\partial \mathbf{L}^{\text{int}}}{\partial \mathbf{u}}\right|_{\mathbf{u}_i^{n-1}} \tag{58}$$

The system to be solved is written finally:

$$\mathbf{K}_i^{n-1} . \delta \mathbf{u}_i^n = \mathbf{L}_i^{\text{méca}} - \mathbf{L}_i^{\text{int},n-1} \tag{59}$$

The vector of the internal forces $\mathbf{L}_i^{\text{int},n-1}$ is calculated starting from the constraints $\boldsymbol{\sigma}_i^{n-1}$. Those being calculated starting from displacements $\mathbf{u}_i^{n-1}$ via the relation of behavior of the material [§1.1]. In fact, in the case of behaviors ***incrémentaux***, $\boldsymbol{\sigma}_i^{n-1}$ is calculated from $(\boldsymbol{\sigma}_{i-1}, \boldsymbol{\alpha}_{i-1})$ and of the increment of deformation $\boldsymbol{\varepsilon}(\Delta \mathbf{u}_i^{n-1})$ induced by the increment of displacement since the beginning of the iterative process (including the phase of prediction) or by the gradient of the transformation $\mathbf{F}$ in the case of great transformations.

2.4.3 Difference of the matrices in prediction and correction

It is important to stress that the tangent matrix resulting from the option `RIGI_MECA_TANG` (phase of prediction) and the tangent matrix resulting from the option `FULL_MECA` (phase of correction) are in general not identical. Let us suppose that one reached convergence for the moment t_{i-1} and that one now seeks to obtain balance for the next moment t_i. The matrix resulting from `RIGI_MECA_TANG` comes from a linearization from equilibrium equations compared to ***time*** around $(\mathbf{u}_{i-1}, \boldsymbol{\lambda}_{i-1})$ *i.e.* around balance at the moment t_{i-1}. It is thus the tangent matrix of the converged system at the moment t_{i-1}.

On the other hand, the matrix resulting from FULL_MECA comes from a linearization of the equilibrium equations compared to ***displacement*** around $\mathbf{u}_i^n$ *i.e.* around balance at the moment t_i.

One can interpret the differences enters RIGI_MECA_TANG and FULL_MECA in other words. One can thus show that the matrix resulting from RIGI_MECA_TANG corresponds to the tangent operator of the problem **continuous** in time, known as also problem of speed (and connects the speed of constraint at the speed of deformation), whereas the matrix resulting from FULL_MECA corresponds to the tangent operator of the problem **discretized** in time. The document [R5.03.02] gives the expression in each of the two cases for the relation of elastoplasticity of Von Mises to isotropic or kinematic work hardening linear.

It is pointed out that the treatment of a relation of behavior [R5.03.02 § 5] consists with:

- To calculate the constraints $\boldsymbol{\sigma}_i^n$ and internal variables $\boldsymbol{\alpha}_i^n$ starting from the initial state $(\boldsymbol{\sigma}_{i-1}, \boldsymbol{\alpha}_{i-1})$ and of the increment of deformation $\boldsymbol{\varepsilon}(\Delta \mathbf{u}_i^{n-1})$ induced by the increment of displacement since the beginning of the iterative process (including the phase of prediction).
- To calculate the internal forces $\mathbf{L}_i^{\text{int},n} = \mathbf{Q}_i^T . \boldsymbol{\sigma}_i^n$.
- To calculate (possibly) the tangent matrix (option RIGI_MECA_TANG for the phase of prediction, option FULL_MECA for the iterations of Newton).

2.5 Convergence criteria

At the end of the prediction and each iteration of Newton, one must estimate if the iterative process converged (the balance of the structure is reached). One places oneself at the step of current time t_i and with the iteration of Newton n (given that the value $n=0$ corresponds to the prediction). There exist four convergence criteria.
The criterion RESI_GLOB_MAXI consist in checking that the infinite standard[2] residue is lower than the value γ specified by the user.

$$\left\| \mathbf{Q}^T . \boldsymbol{\sigma}_i^n - \mathbf{L}_i^{\text{méca}} \right\|_\infty \leq \gamma \tag{60}$$

It is not advised to use this criterion alone, because one cannot easily have an idea of the acceptable orders of magnitude absolute.

The criterion RESI_GLOB_RELA (selected by default) amounts checking that the residue is sufficiently small, like previously, and this compared to a quantity representative of the loading.

$$\frac{\left\| \mathbf{Q}^T . \boldsymbol{\sigma}_i^n - \mathbf{L}_i^{\text{méca}} \right\|_\infty}{\left\| \mathbf{L}_i^{\text{méca}} + \mathbf{L}_i^{\text{varc}} \right\|_\infty} \leq \eta \tag{61}$$

η being desired relative precision given by the user under the keyword RESI_GLOB_RELA (or the value by default of 10^{-6}).
One can notice that, in the case of use of RESI_GLOB_RELA, the criterion can become singular if the external loading $\mathbf{L}_i^{\text{méca}} + \mathbf{L}_i^{\text{varc}}$ becomes null. This can arrive in the event of total discharge of the structure. If such a case arises (i.e loading 10^{-6} time smaller than the smallest loading observed until this increment), the code uses the criterion then RESI_GLOB_MAXI with like value that observed with the convergence of the preceding increment. When the loading becomes again not no one, one returns to the initial criterion.

The third criterion is the criterion RESI_REFE_RELA : the idea of this criterion is to build a nodal force of reference, which will be used to estimate term in the long term, the nullity (approximate) of the residue:

$$\forall\, j \in (\text{ddl}) \qquad \left| \left(\mathbf{Q}^T . \boldsymbol{\sigma}_i^n - \mathbf{L}_i^{\text{méca}} \right)_j \right| \leq \varepsilon \, . \mathbf{F}_j^{\text{ref}} \tag{62}$$

More precisely, the nodal force of reference $\mathbf{F}_j^{\text{ref}}$ is built starting from the data of an amplitude of reference A^{ref} who can be:

- A constraint;

2 The infinite standard corresponds simply to the maximum component of the absolute value of the vector

- A pressure, a temperature in the case of the THM;
- A force generalized in the case as of beams or of the hulls;
- others…

The list is accessible in documentation from use of the order STAT_NON_LINE [U4.51.03], description of the operand RESI_REFE_RELA.

If one takes as example a constraint, the amplitude of reference σ^{ref} being given by the user via the keyword SIGM_REFE . From this amplitude of constraint of reference, one defines the tensor $\boldsymbol{\sigma}^{\text{test}}$: it is null for all these components, except *J*- ième which is worth σ^{ref} . One defines then, for each node of each element the nodal force $\tilde{R}_i^e$ (the goal being to give an idea of the importance of a component in a point of Gauss of the constraint on the nodal force):

$$\tilde{R}_i^e = \frac{1}{N} . \sum_{\alpha=1}^{N} \sum_{j=1}^{M} | B_{i,j}^{\alpha} . \sigma_j^{\text{test}} | . \omega^{\alpha} \tag{63}$$

With N the number of points of Gauss of the element, M the component count of the tensor of the constraints; the exhibitor α being used to note the evaluation of quantity at the point of Gauss. For example ω^{α} are the weights of the points of Gauss.

Note: For certain elements, as the bars, the grids or the membranes, this definition leads to worthless residues of reference on certain axes. To cure it, one determines the nodal forces of reference via a calculation of order of magnitude based on the size of the element.

The nodal force of reference is then defined by:

$$\mathbf{F}_i^{\text{ref}} = \min_{e \in \Gamma_i} \tilde{R}_i^e \tag{64}$$

where Γ_i is the whole of the elements connected to the node i .

The fourth criterion is the criterion RESI_COMP_RELA : the idea of this criterion is to separate the various component contributions of the residue by components (to the direction DX, DY, DZ, PRE1, PRE2, TEMP). Each vector obtained will be then normalized by the force interns correspondent with this residue. This choice of convergence criteria has direction only for the strongly evolutionary problems, typically problems THM. Who more is, this choice will be effective since one will have problems with strong contrasts. In fact indeed the zones with “strong gradient” will control convergence. One defines $\mathbf{F}^n(c)$ the part of the residue $\mathbf{Q}^T . \boldsymbol{\sigma}_i^n - \mathbf{L}_i^{\text{méca}}$ corresponding to the component c and $\mathbf{L}^{\text{int},0}(c)$ the vector of the internal forces in prediction correspondent with this same component c . The criterion RESI_COMP_RELA cost then to check that this residue is sufficiently small, i.e.:

$$\max_{c=1,\ldots,nbcmp} \left(\frac{\max_{d=1,\ldots,nbddl} |\mathbf{F}^n(c,d)|}{\max_{d=1,\ldots,nbddl} |\mathbf{L}^{\text{int},0}(c,d)|} \right) < \varepsilon \tag{65}$$

Convergence is issued carried out when all the criteria specified by the user are checked simultaneously. By default, one makes a test on the relative total residue (RESI_GLOB_RELA) and the maximum number of iterations of Newton (ITER_GLOB_MAXI).

For the residues RESI_GLOB_RELA and RESI_GLOB_MAXI , all the components of the field of displacement are used in the evaluation of the standard $\|.\|_{\infty}$, except in two cases where a particular treatment is made on the level of the choice of the components:

- For the loadings of the type AFFE_CHAR_CINE , the degree of freedom concerned is ignored in the evaluation of the standard of the residue because the procedure of elimination of the unknown factors does not make it possible to reach the reactions of supports;

- For the continuous contact, the components LAGR_C and LAGR_F1/LAGR_F2 are ignored in the evaluation of the standard because the law of Signorini-Coulomb is already checked in the algorithm (see [R5.03.52]) and that these terms are dimensionally incoherent with those relating to displacements; On the other hand, for the case of the contact in XFEM, these components are preserved because they are used to check condition LBB;

2.6 Use of an evolutionary matrix tangent-secant

The method described in this paragraph applies exclusively to the strongly non-linear problems, where a method of Newton classical fails for any type of choice of matrix, for the phase of prediction or correction. Typically, the usual method of Newton is put at fault for the problems badly-posed coming from the use of the lenitive laws of behavior (see for example R5.04.01) .

In these situations, a not-convergence appears when the algorithm does not manage to choose between several acceptable solutions, in an increment of (pseudonym) - time given. This defect of convergence at the total level is generally translated at the local level (i.e at the point of integration) by an alternation repeated between a non-dissipative state (elastic) and a dissipative state (plasticity, damage,…) during consecutive iterations of Newton.

One of the strategies consists in using the concept of piloting (see R5.03.80) to mitigate the insufficiencies of Newton. The other strategy consists in modifying the tangent matrix. It is this last strategy which one details here.

While following the state of each point of integration of one iteration to the other, one can locate the points responsible for a total not-convergence. Once these located points, one decides to modify the matrix by hoping that this modification will allow a total convergence.

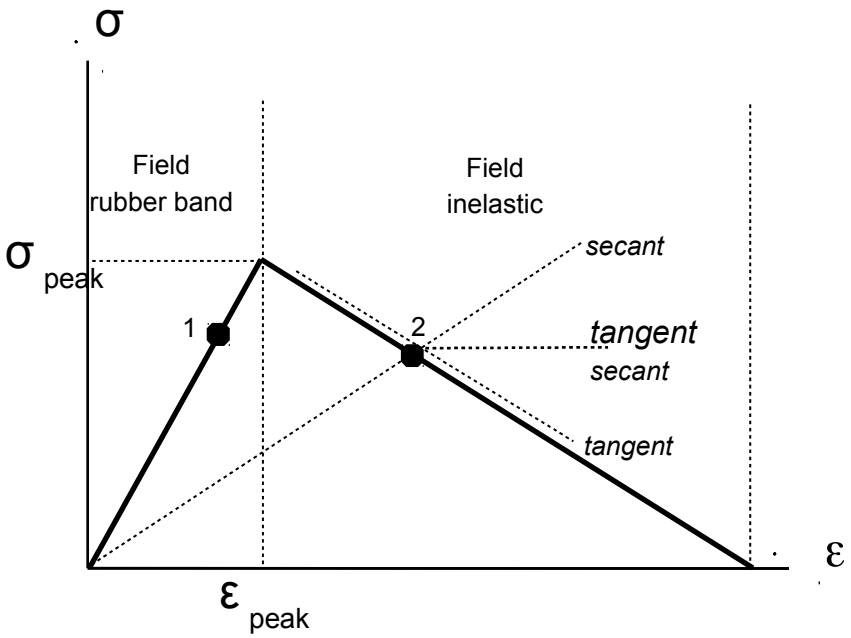

Figure 2-2.6-a: Law of behavior lenitive, use of a mixed matrix tangent-secant

Baptized approach tangent-secant, activated under the keyword BEHAVIOR with TANGENTE_SECANTE='OUI', justifies itself by the following reasoning: if the method of Newton using the coherent tangent matrix does not converge, it is often because a certain number (variable) of points integration state (non-dissipative/dissipative) between two total iterations of Newton changes. At the local level (see Figure 2-2.6-a), that wants to say that one continues to alternate between field 1 ($\varepsilon < \varepsilon_{pic}$) and field 2 ($\varepsilon > \varepsilon_{pic}$). Because of the break of slope between 1 and 2, the use of a secant or tangent matrix coherent leads to a very poor

approximation, from where interest to modify it. The choice which one present consists in building the tangent matrix like a linear combination between the coherent tangent matrix and the secant matrix, both being determined by the laws of behavior. Currently, the approach is available only for the lenitive law of behavior ENDO_ISOT_BETON.

To manage the starting of the option tangent-secant, one introduces an additional internal variable compared to the existing internal variables, $\boldsymbol{\alpha}=(\alpha_1,\ldots\alpha_n,\alpha_{n+1})$ (with n the number of internal variables of the model used). This variable represents possible alternation between the elastic state and the lenitive state of a point of Gauss. One initializes it with the first iteration of Newton of each new step of time, then one makes it evolve to know, in each point of Gauss, the number of successive alternations between the two states. By having this information, one can estimate that starting from a certain threshold (for example $S_0=3$ alternations), the algorithm of Newton will not be able to converge any more for the increment of current time and which it is necessary to modify the tangent matrix. To modify the matrix, one is based directly on the way in which the coherent tangent matrix in ENDO_ISOT_BETON is built (see [R7.01.04]). It is a question of making the sum between the dissipative part and the nondissipative part.

$$\mathbf{K}_{\text{tg}}=\mathbf{K}_{\text{sc}}+\mathbf{K}_{\text{end}} \tag{66}$$

where $\mathbf{K}_{\text{tg}}$ is the tangent matrix, $\mathbf{K}_{\text{sc}}$ the secant matrix (left non-dissipative) and $\mathbf{K}_{\text{end}}$ damaging correction (left dissipative). For the modified matrix $\mathbf{K}_{\text{t-s}}$, the expression is replaced $\mathbf{K}_{\text{tg}}$ in (66) by:

$$\mathbf{K}_{\text{t-s}}=\mathbf{K}_{\text{sc}}+\eta.\mathbf{K}_{\text{end}} \tag{67}$$

where η is a function of α_{n+1} with values between 0 and 1. The function η retained in the continuation is the following one:

$$\eta=\frac{1}{A^{(\alpha_{n+1}-S_0)}} \tag{68}$$

where A is a constant and S_0 the threshold on the value amongst successive alternations undergone from which the tangent matrix is modified. For $\alpha_{n+1}=S_0$ the matrix remains tangent coherent and for $\alpha_{n+1}\gg S_0$, it becomes secant. Values considered to be satisfactory for these parameters are $A=1{,}5$ and $S_0=3$ (values by default). The choice on the evolution of the value of α_{n+1} is paramount for the performance of the algorithm. One chooses an increase in α_{n+1} of $G=1{,}0$, $\alpha_{n+1}\rightarrow\alpha_{n+1}+G$ for each new alternation enters an elastic state and a damaging state, then a reduction in α_{n+1} of P, $\alpha_{n+1}\rightarrow\alpha_{n+1}-P$, when the state remains damaging twice continuation. The objective of the use of P is to allow the return to the coherent tangent matrix when a point of Gauss remains damaging on several iterations, since the coherent tangent matrix makes convergence quadratic, provided that one is close to the solution. The value of the rate of reduction P compared to the rate of increase G, is crucial for the behavior of the evolutionary algorithm. The total idea consists in increasing α_{n+1}, when one is far from the solution to have an operator closer to secant than of tangent coherent, then once “near” to the solution, to rock out of coherent tangent matrix (which is the best within the meaning of Newton). The report P/G (keyword TAUX_RETOUR – 0.05 by default) represents the third parameter of the algorithm, besides A (keyword AMPLITUDE) and S_0 (keyword THRESHOLD).

2.7 Method of Newton-Krylov

2.7.1 Principle general

The method of Newton-Krylov is part of the inaccurate methods of Newton. It is only usable when the solvor of the linear system (59) is iterative (in opposition to a direct solvor). This approach does not modify the choice of the tangent matrix of the system like the preceding methods. She exploits the convergence criteria of the iterative solvor used for the linearized system. By adapting the criterion as well as possible of convergence of the iterative method to convergence of Newton, one avoids making useless iterations (in the linear solvor) and one gains thus in computing times.

2.7.2 Implementation

The principle general of the inaccurate methods of Newton is to replace the condition that the increment of solution $\delta \mathbf{u}_i^n$ that is to say the exact solution of the system (59) by a weaker condition. It is asked that $\delta \mathbf{u}_i^n$ check the condition:

$$\left\| \mathbf{K}_i^{n-1} . \delta \mathbf{u}_i^n - \left(\mathbf{L}_i^{\text{méca}} - \mathbf{L}_i^{\text{int},n-1} \right) \right\| \leqslant \eta_n \left\| \mathbf{L}_i^{\text{méca}} - \mathbf{L}_i^{\text{int},n-1} \right\| \quad (69)$$

where η_n it is called *sustained pressure term*.

One can show that the method suggested is convergent and that when the continuation η_n tends towards 0, convergence is super-linear (see [8] p.96). The smaller this value is, the more the solution will be close to that obtained by an exact resolution, but less one will save time with the resolution of the linear system. It is thus necessary to find a good compromise between solving the linear systems quickly and not too much not to degrade the convergence of the iterations of Newton.
By examining the condition (69), it is noted that it is identical to the relative convergence criteria of the iterative solveurs used to solve the linearized system of Newton. To check this condition, it is thus a question of using it *sustained pressure term* like convergence criteria of an iterative linear solvor.

As one saw previously, it as should be made sure as the continuation η_n tends towards 0 to preserve the super-linear convergence of the method of Newton. With this intention, one will control η_n with the decrease of the residue of Newton by the law of evolution (*cf.* [8] p.105):

$$\eta_{n+1}^{Res} = \gamma \frac{\left\| \mathbf{R}_i^n \right\|^2}{\left\| \mathbf{R}_i^{n-1} \right\|^2} \quad (70)$$

where the constant is selected such as $\gamma = 0.1$.

This simple formula is not sufficient in practice because it is necessary to guarantee an adequate decrease of η_n . For that, one determines completely η_n by the following expression:

$$\eta_{n+1} = \begin{cases} \eta_0 & n = -1 \\ max\left(min\left(0.4\,\eta_n, \eta_{n+1}^{Res}\right), \eta_{min} \right) & n \geqslant 0, \quad (1-\gamma)\eta_n^2 \leqslant 0.2 \\ min\left(0.4\,\eta_n, max\left(\eta_{n+1}^{Res}, (1-\gamma)\eta_n^2\right)\right) & n \geqslant 0, \quad (1-\gamma)\eta_n^2 > 0.2 \end{cases} \quad (71)$$

where the constant is worth $\eta_0 = 0.9$ and corresponds to the convergence criteria used for the first linear resolution.
η_{min} , as for it, is the value of the convergence criteria of the iterative linear solvor provided by the user (keyword RESI_RELA).

3 Limiting conditions and loadings

3.1 Classification

In the following paragraphs, we will describe the whole of the possible loadings in the operator and their classification. Initially, it is advisable to distinguish three main categories of loadings:

- The loadings of Dirichlet (limiting conditions) apply to the nodal unknown factors in the broad sense: it can be a displacement, a temperature or a pressure (for the THM). They can be applied by elimination (AFFE_CHAR_CINE) or by dualisation (AFFE_CHAR_MECA). When the limiting conditions are treated by elimination, their taking into account is done at the time of the resolution of the linear system, in manner interns and thus does not modify at all the equations already described précdemment;
- The loadings of Neumann apply in general to flows. They are conditions in efforts, in general, definite on the meshs (except for the loading FORCE_NODALE).

There is another distinction to realize between the loadings ***follower*** and those which are not it. A loading is following when it depends on the geometry of the structure. Typically, the pressure is exerted in the direction opposed to the normal. Therefore, when the structure becomes deformed with the evolution of the load, the loading, expressed in an absolute reference mark, is transformed. There exist also following loadings of Dirichlet. In fact limiting conditions depend on the geometry because they are non-linear. The loads which do not depend on the geometry of the structure are called dead or fixed loads (for example, gravity).

3.2 Chargements following

To indicate that a load must be treated like a following load in STAT_NON_LINE, one indicates TYPE_CHARGE='SUIV' under the keyword EXCIT. A mechanical loading $\mathbf{L}_i^{\text{méca}}(\mathbf{u}_i)$ comprising following loads thus breaks up into two parts:

$$\mathbf{L}_i^{\text{méca}}(\mathbf{u}_i)=\mathbf{L}_i^{\text{fixe}}+\mathbf{L}_i^{\text{suiv}}(\mathbf{u}_i) \tag{72}$$

The exhibitor $^{\text{fixe}}$ indicate the died loads here, and $^{\text{suiv}}$ following loads. The system of equations to be solved becomes then:

$$\mathbf{L}_i^{\text{int}}=\mathbf{L}_i^{\text{fixe}}+\mathbf{L}_i^{\text{suiv}}(\mathbf{u}_i) \tag{73}$$

The operations of derivation making it possible to write the phase of prediction and the iterations of the method of Newton thus utilize the derivative of $\mathbf{L}_i^{\text{suiv}}(\mathbf{u}_i)$ compared to displacements $(\mathbf{u}_i)$.The phase of prediction becomes:

$$\left(\mathbf{K}_{i-1}-\left.\frac{\partial \mathbf{L}^{\text{suiv}}}{\partial \mathbf{u}}\right|_{\mathbf{u}_i^{n-1}}\right).\Delta \mathbf{u}_i^0=\Delta \mathbf{L}_i^{\text{fixe}}+\Delta \mathbf{L}_i^{\text{suiv}}+\Delta \mathbf{L}_i^{\text{varc}} \tag{74}$$

And the iterations of Newton consist in solving the system:

$$\left(\mathbf{K}_i^{n-1}-\left.\frac{\partial \mathbf{L}^{\text{suiv}}}{\partial \mathbf{u}}\right|_{\mathbf{u}_i^{n-1}}\right).\delta \mathbf{u}_i^n=\mathbf{L}^{\text{fixe}}+\mathbf{L}_i^{\text{suiv},n-1}(\mathbf{u}_i)-\mathbf{L}_i^{\text{int},n-1} \tag{75}$$

Thus, at the beginning of each step of load (prediction) and with each iteration of Newton, one must calculate a matrix of rigidity $\left.\frac{\partial \mathbf{L}^{\text{suiv}}}{\partial \mathbf{u}}\right|_{\mathbf{u}}$ and a vector $\mathbf{L}^{\text{suiv}}$ dependent on the following loadings.

The only loads of Neumann which can be treated like following loads in the actual position of the operator STAT_NON_LINE are:

- Pressure for modelings 3D, 3D_SI, D_PLAN, D_PLAN_SI, AXIS, AXIS_SI, C_PLAN, C_PLAN_SI [R3.03.04] and COQUE_3D [R3.03.07];
- The loading of gravity for the elements CABLE_POULIE [R3.08.05], elements with three nodes comprising a pulley and two bits of cables: the force of gravity being exerted on the element depends on the respective lengths of the two bits;
- The centrifugal force in great displacements, which for a number of revolutions $\boldsymbol{\omega}$ is given by: $\int_\Omega \rho.\boldsymbol{\omega}\wedge[\boldsymbol{\omega}\wedge\mathbf{OM}].d\Omega = \int_\Omega \rho.\boldsymbol{\omega}\wedge[\boldsymbol{\omega}\wedge(\mathbf{OM_0}+\mathbf{u})].d\Omega$. Available for modelings 3D and AXIS_FOURIER;

- The loading of gravity for all modelings THM unsaturated porous environments [R7.01.10]: indeed, the density depends on the nodal variables to take account of the relations of behavior of the géomatériaux one.

3.3 COdualized limiting nditions – linear Case

We now will take into account the limiting conditions dualized in the writing of the linear system to solve. Initially, we only will consider relations ***linear***. ON supposes the existence of a potential $J(v)$ such as the minimization of this last makes it possible to express the mechanical balance (with the weak direction) of the structure. If $J(u)$ then one is this minimum a:

$$\begin{aligned}&\text{Trouver } u\in V \text{ tel que :}\\&\begin{cases}J(u)=\min\limits_{v\in V} J(v)\equiv\{L^{\text{int}}(u,v)-L^{\text{ext}}(u,v)\}\\ \text{Avec : } V=\{v\in R^n \text{ tel que } Bv=0\}\end{cases}\end{aligned} \tag{76}$$

- $L^{\text{int}}(u,v)$ indicate the sum of the discretized internal forces. It depends on the solution sought via the laws of behavior, kinematics of great transformations, etc.
- $L^{\text{ext}}(u,v)$ indicate the sum of the discretized external forces. It can in the case of depend on the solution like the following forces, of the contact, etc.
- V indicate the whole of the acceptable solutions tests;
- U indicate the whole of the acceptable required solutions;
- B is an operator *linear* space of the fields of displacements on a space of functions defined on part of the edge of the structure;

Note: in mechanics, one can consider the presence of dissipative forces related on the viscous character of the law of behavior or to the forces of friction. In these cases the potential is replaced by the existence of a pseudopotential of dissipation. One does not return in the details but it is shown that one can bring back oneself within the framework of a problem of optimization thanks to the transformation of Legendre-Fenchel. By preoccupation with a simplicity, one keeps the framework general of the preceding equation because the continuation of the developments is not impacted by the existence of a pseudopotential.

In discrete form, the dualisation of the boundary conditions of Dirichlet $\mathbf{B}.\mathbf{u}=\mathbf{u}^d(t)$ conduit with the following problem [R3.03.01]:

$$\begin{cases}\mathbf{L}^{\text{int}}(\mathbf{u},t)+\mathbf{B}^T.\boldsymbol{\lambda}=\mathbf{L}^{\text{ext}}(t)\\ \mathbf{B}.\mathbf{u}=\mathbf{u}^d(t)\end{cases} \tag{77}$$

The unknown factors are now, at any moment t, the couple $(\mathbf{u},\boldsymbol{\lambda})$, where $\boldsymbol{\lambda}$ represent them *multipliers of Lagrange* boundary conditions of Dirichlet [R3.03.01]. The vector $\mathbf{B}^{\mathbf{T}}.\lambda$ be interpreted like the opposite of the reactions of support to the corresponding nodes. While parameterizing by the moment t_i :

$$\begin{cases}\mathbf{L}_i^{\text{int}}+\mathbf{B}^T.\boldsymbol{\lambda}_i=\mathbf{L}_i^{\text{ext}}\\ \mathbf{B}.\mathbf{u}_i=\mathbf{u}_i^d\end{cases} \tag{78}$$

To find balance thus consists in cancelling in $(\mathbf{u}_i,\boldsymbol{\lambda}_i,t_i)$ the vector residue of balance which will be defined by:

$$\mathbf{R}_i(\mathbf{u}_i,\boldsymbol{\lambda}_i,t_i)=\begin{pmatrix}\mathbf{L}_i^{\text{int}}+\mathbf{B}^{\mathbf{T}}.\boldsymbol{\lambda}_i-\mathbf{L}_i^{\text{ext}}\\ \mathbf{B}.\mathbf{u}_i-\mathbf{u}_i^d\end{pmatrix} \tag{79}$$

The unknown factors are calculated in an incremental way by the total algorithm of resolution including the multipliers of Lagrange of the dualized limiting conditions. From $(\mathbf{u}_{i-1},\boldsymbol{\lambda}_{i-1})$, solution satisfying balance in t_{i-1}, one determines $\Delta\mathbf{u}_i$ and $\Delta\boldsymbol{\lambda}_i$ who will allow to obtain the solution in t_i :

$$\begin{cases}t_i=t_{i-1}+\Delta t_i\\ \mathbf{u}_i=\mathbf{u}_{i-1}+\Delta\mathbf{u}_i\\ \boldsymbol{\lambda}_i=\boldsymbol{\lambda}_{i-1}+\Delta\boldsymbol{\lambda}_i\end{cases} \tag{80}$$

3.3.1 Phase of prediction of Euler

For the prediction, the system always should be linearized (77) compared to time but, in this case, around the two unknown factors (displacements and multipliers of Lagrange) $(\mathbf{u}_{i-1}, \boldsymbol{\lambda}_{i-1})$. It is noted initially that the linearization of the reactions of support $\mathbf{B}^T.\boldsymbol{\lambda}_i$ is immediate because one considers linear limiting conditions and thus the matrix $\mathbf{B}$ is constant (it does not depend on displacements or time). Like $\boldsymbol{\lambda}_i = \Delta\boldsymbol{\lambda}_i^0 + \boldsymbol{\lambda}_{i-1}$, it comes immediately:

$$\mathbf{B}^T.\boldsymbol{\lambda}_i = \mathbf{B}^T.\Delta\boldsymbol{\lambda}_i^0 + \mathbf{B}^T.\boldsymbol{\lambda}_{i-1} \tag{81}$$

It is supposed that the mechanical loading does not depend on time (the following loads are excluded) and that the limiting conditions of Dirichlet are also linear, therefore:

$$\begin{cases} \mathbf{L}_i^{\text{méca}} = \mathbf{L}_{i-1}^{\text{méca}} + \Delta\mathbf{L}_i^{\text{méca}} \\ \mathbf{u}_i^d = \mathbf{u}_{i-1}^d + \Delta\mathbf{u}_i^d \end{cases} \tag{82}$$

One obtains for the equilibrium equation:

$$\mathbf{L}_{i-1}^{\text{int}} + \left.\frac{\partial\mathbf{L}^{\text{int}}}{\partial\mathbf{u}}\right|_{\mathbf{u}_{i-1}}.\Delta\mathbf{u}_i^0 + \left.\frac{\delta\mathbf{L}^{\text{int}}}{\delta t}\right|_{t_{i-1}}.\Delta t_i + \mathbf{B}^T.\Delta\boldsymbol{\lambda}_i^0 + \mathbf{B}^T.\boldsymbol{\lambda}_{i-1} = \mathbf{L}_{i-1}^{\text{méca}} + \Delta\mathbf{L}_i^{\text{méca}} \tag{83}$$

There is balance at the moment t_{i-1}, i.e.:

$$\mathbf{L}_{i-1}^{\text{int}} + \mathbf{B}^T.\boldsymbol{\lambda}_{i-1} = \mathbf{L}_{i-1}^{\text{méca}} \tag{84}$$

And it thus remains:

$$\left.\frac{\partial\mathbf{L}^{\text{int}}}{\partial\mathbf{u}}\right|_{\mathbf{u}_{i-1}}.\Delta\mathbf{u}_i^0 + \left.\frac{\delta\mathbf{L}^{\text{int}}}{\delta t}\right|_{t_{i-1}}.\Delta t_i + \mathbf{B}^T.\Delta\boldsymbol{\lambda}_i^0 = \Delta\mathbf{L}_i^{\text{méca}} \tag{85}$$

If one now looks at the second equation of the system (77), one obtains for the limiting conditions of Dirichlet:

$$\mathbf{B}.(\mathbf{u}_{i-1} + \Delta\mathbf{u}_i^0) = \mathbf{u}_{i-1}^d + \Delta\mathbf{u}_i^d \tag{86}$$

There is balance at the moment t_{i-1}, i.e.:

$$\mathbf{B}.\mathbf{u}_{i-1} = \mathbf{u}_{i-1}^d \tag{87}$$

It remains finally:

$$\mathbf{B}.\Delta\mathbf{u}_i^0 = \Delta\mathbf{u}_i^d \tag{88}$$

One obtains the system of equations allowing to calculate predictive values $(\Delta\mathbf{u}_i^0, \Delta\boldsymbol{\lambda}_i^0)$:

$$\begin{cases} \mathbf{K}_{i-1}.\Delta\mathbf{u}_i^0 + \mathbf{B}^T.\Delta\boldsymbol{\lambda}_i^0 = \mathbf{L}_i^{\text{méca}} - \mathbf{Q}_{i-1}^T.\boldsymbol{\sigma}_{i-1} - \mathbf{B}^T.\boldsymbol{\lambda}_{i-1} + \Delta\mathbf{L}_i^{\text{varc}} \\ \mathbf{B}.\Delta\mathbf{u}_i^0 = \Delta\mathbf{u}_i^d \end{cases} \tag{89}$$

It will be noticed whereas this expression utilized from now on the multipliers of Lagrange at the moment *precedent*, which is sometimes unknown (with the first increment of load, for example). What wants to say that with this new expression, one moved the problem of the knowledge of the internal forces at the moment t_{i-1} towards the ignorance of the multipliers of Lagrange at this same moment! But as the limiting conditions are linear, the problem is simplified. Let us consider that the solution of (89) with regard to the multipliers of Lagrange $\hat{\boldsymbol{\lambda}}_i$ is written in incremental form:

$$\hat{\boldsymbol{\lambda}}_i = \hat{\boldsymbol{\lambda}}_{i-1} + \Delta\hat{\boldsymbol{\lambda}}_i \tag{90}$$

This solution solves the first equation of the system:

$$\mathbf{K}_{i-1}.\Delta\mathbf{u}_i^0 + \mathbf{B}^T.\Delta\hat{\boldsymbol{\lambda}}_i^0 = \mathbf{L}_i^{\text{méca}} - \mathbf{Q}_{i-1}^T.\boldsymbol{\sigma}_{i-1} - \mathbf{B}^T.\hat{\boldsymbol{\lambda}}_{i-1} + \Delta\mathbf{L}_i^{\text{varc}} \tag{91}$$

The idea is to search it $\hat{\boldsymbol{\lambda}}_i$. Like the operator $\mathbf{B}^T$ is constant, while applying 90, one a:

$$\mathbf{K}_{i-1}.\Delta\mathbf{u}_i^0 + \mathbf{B}^T.\hat{\boldsymbol{\lambda}}_i = \mathbf{L}_i^{\text{méca}} - \mathbf{Q}_{i-1}^T.\boldsymbol{\sigma}_{i-1} + \Delta\mathbf{L}_i^{\text{varc}} \tag{92}$$

It is supposed that the limiting conditions are checked, therefore:

$$\mathbf{B}.\Delta\mathbf{u}_i^0=\Delta\mathbf{u}_i^d \tag{93}$$

Imposed displacements are also written in incremental form:

$$\mathbf{u}_i^d=\mathbf{u}_{i-1}^d+\Delta\mathbf{u}_i^d \tag{94}$$

The matrix $\mathbf{B}$ is constant, we thus had with the preceding increment (the problem was solved):

$$\mathbf{B}.\mathbf{u}_{i-1}=\mathbf{u}_{i-1}^d \tag{95}$$

While using 94 and 95 in 93 :

$$\mathbf{B}.\Delta\mathbf{u}_i^0=\Delta\mathbf{u}_i^d=\mathbf{u}_i^d-\mathbf{u}_{i-1}^d=\mathbf{u}_i^d-\mathbf{B}.\mathbf{u}_{i-1} \tag{96}$$

With balance, one thus has $\hat{\boldsymbol{\lambda}}_i$ who satisfies also the limiting conditions which one rewrites:

$$\mathbf{B}.\Delta\mathbf{u}_i^0=\mathbf{u}_i^d-\mathbf{B}.\mathbf{u}_{i-1} \tag{97}$$

The vector of the multipliers of Lagrange $\hat{\boldsymbol{\lambda}}_i$ can thus be found at the time of the phase of prediction by modifying the equation of imposition of the limiting conditions by the expression 97. By analogy with the increment of the displacements found in prediction $\Delta\mathbf{u}_i^0$ one will note $\Delta\boldsymbol{\lambda}_i^0=\hat{\boldsymbol{\lambda}}_i$:

$$\begin{cases}\mathbf{K}_{i-1}.\Delta\mathbf{u}_i^0+\mathbf{B}^T.\Delta\boldsymbol{\lambda}_i^0=\mathbf{L}_i^{\text{méca}}-\mathbf{Q}_{i-1}^T.\boldsymbol{\sigma}_{i-1}+\Delta\mathbf{L}_i^{\text{varc}}\\ \mathbf{B}.\Delta\mathbf{u}_i^0=\mathbf{u}_i^d-\mathbf{B}.\mathbf{u}_{i-1}\end{cases} \tag{98}$$

A typical case relates to the use of an excitation of the type TYPE_CHARGE= 'DIDI'meaning differential Dirichlet, i.e. compared to the initial state. That consists, for the boundary conditions of the blockings type, to impose, not $\mathbf{B}.\mathbf{u}=\mathbf{u}^d$, but $\mathbf{B}.(\mathbf{u}-\mathbf{u}_{\text{didi}})=\mathbf{u}^d$ In this case, the system to be solved in the phase of prediction for the new increment of load is:

$$\begin{cases}\mathbf{K}_{i-1}.\Delta\mathbf{u}_i^0+\mathbf{B}^T.\Delta\boldsymbol{\lambda}_i^0=\mathbf{L}_i^{\text{méca}}-\mathbf{Q}_{i-1}^T.\boldsymbol{\sigma}_{i-1}+\Delta\mathbf{L}_i^{\text{varc}}\\ \mathbf{B}.\Delta\mathbf{u}_i^0=\mathbf{u}_i^d-\mathbf{B}.\mathbf{u}_{i-1}+\mathbf{B}.\mathbf{u}_{\text{didi}}\end{cases} \tag{99}$$

3.3.2 Phase of correction of Newton

One must linearize the system 26 compared to the unknown factors in $(\mathbf{u}_i^n,\boldsymbol{\lambda}_i^n)$ with t_i constant. One starts by linearizing the internal forces $\mathbf{L}_i^{\text{int},n}$:

$$\mathbf{L}_i^{\text{int},n}\approx\mathbf{L}_i^{\text{int},n-1}+\left.\frac{\partial\mathbf{L}^{\text{int}}}{\partial\mathbf{u}}\right|_{\mathbf{u}_i^{n-1}}.\delta\mathbf{u}_i^n \tag{100}$$

Linearization of the reactions of support $\mathbf{B}^T.\boldsymbol{\lambda}_i^n$ is immediate (linear conditions):

$$\mathbf{B}^T.\boldsymbol{\lambda}_i^n=\mathbf{B}^T.\boldsymbol{\lambda}_i^{n-1}+\mathbf{B}^T.\delta\boldsymbol{\lambda}_i^n \tag{101}$$

It is supposed that the mechanical loading does not depend on time (the following loads are excluded) and that the limiting conditions of Dirichlet are also linear. One obtains for the equilibrium equation:

$$\mathbf{L}_i^{\text{int},n-1}+\left.\frac{\partial\mathbf{L}^{\text{int}}}{\partial\mathbf{u}}\right|_{\mathbf{u}_i^{n-1}}.\delta\mathbf{u}_i^n+\mathbf{B}^T.\boldsymbol{\lambda}_i^{n-1}+\mathbf{B}^T.\delta\boldsymbol{\lambda}_i^n=\mathbf{L}_i^{\text{méca}} \tag{102}$$

For the limiting conditions, the linearization of the system (77) we gives in a way similar to 97:

$$\mathbf{B}.\delta\mathbf{u}_i^n=\mathbf{u}_i^d-\mathbf{B}.\mathbf{u}_i^{n-1} \tag{103}$$

The system to be solved is written finally:

$$\begin{cases}\mathbf{K}_i^{n-1}.\delta\mathbf{u}_i^n+\mathbf{B}^T.\delta\boldsymbol{\lambda}_i^n=\mathbf{L}_i^{\text{méca}}-\mathbf{L}_i^{\text{int},n-1}-\mathbf{B}^T.\boldsymbol{\lambda}_i^{n-1}\\ \mathbf{B}.\delta\mathbf{u}_i^n=\mathbf{u}_i^d-\mathbf{B}.\mathbf{u}_i^{n-1}\end{cases} \tag{104}$$

3.3.3 Adaptation of the convergence criteria

One clarifies the adaptation here of RESI_GLOB_MAXI and RESI_GLOB_RELA with the cases of the dualized limiting conditions. The criterion RESI_GLOB_MAXI consist in checking that the infinite standard of the residue is lower than the value γ specified by the user. It is necessary to introduce the contribution of the dualized limiting conditions:

$$\|\mathbf{Q}^T.\boldsymbol{\sigma}_i^n+\mathbf{B}^T.\lambda_i^n+-\mathbf{L}_i^{\text{méca}}\|_\infty \leq \gamma \tag{105}$$

•The criterion RESI_GLOB_RELA (selected by default) amounts checking that the residue is sufficiently small, like previously, and this compared to a quantity representative of the loading.

$$\bullet\ \frac{\|\mathbf{Q}^T.\boldsymbol{\sigma}_i^n+\mathbf{B}^T.\lambda_i^n-\mathbf{L}_i^{\text{méca}}\|_\infty}{\|\mathbf{L}_i^{\text{méca}}+\mathbf{L}_i^{\text{varc}}+\mathbf{B}^T.\lambda_i^n\|_\infty}\leq\eta \qquad \bullet \tag{106}$$

3.4 COdualized limiting nditions – non-linear Case

Now let us consider the case of dualized limiting conditions non-linear. For example, LIAISON_SOLIDE in great transformations. ON supposes the existence of a potential $J(v)$ such as the minimization of this last makes it possible to express the mechanical balance (with the weak direction) of the structure. If $J(u)$ then one is this minimum a:

$$\left\{\begin{array}{l}\text{Trouver } u\in V \text{ tel que :}\\ \quad J(u)=\min_{v\in V} J(v)\equiv\{L^{\text{int}}(u,v)-L^{\text{ext}}(u,v)\}\\ \quad \text{Avec : } V=\{v\in R^n \text{ tel que } Bv=0 \text{ et } C(v)=0\}\end{array}\right. \tag{107}$$

- $L^{\text{int}}(u,v)$ indicate the sum of the discretized internal forces. It depends on the solution sought via the laws of behavior, kinematics of great transformations, etc.
- $L^{\text{ext}}(u,v)$ indicate the sum of the discretized external forces. It can in the case of depend on the solution like the following forces, of the contact, etc.
- V indicate the whole of the acceptable solutions tests;
- U indicate the whole of the acceptable required solutions;
- B is an operator *linear* space of the fields of displacements on a space of functions defined on part of the edge of the structure;
- $C(v)$ is an operator *non-linear* space of the fields of displacements on a space of functions defined on part of the edge of the structure;

Non-linear limiting conditions, one considers the example illustrated on the figure (4.3-1), it is wanted that the solid remains rigid, i.e. the distance enters the node M is related to the other nodes M_i remain constant. That is to say:

$$C(u_{M_i}-u_M)=\sqrt{\left(x_{\vec{e}_x M_i}-x_{\vec{e}_x M}\right)^2+\left(x_{\vec{e}_y M_i}-x_{\vec{e}_y M}\right)^2+\left(x_{\vec{e}_z M_i}-x_{\vec{e}_z M}\right)^2} \tag{108}$$

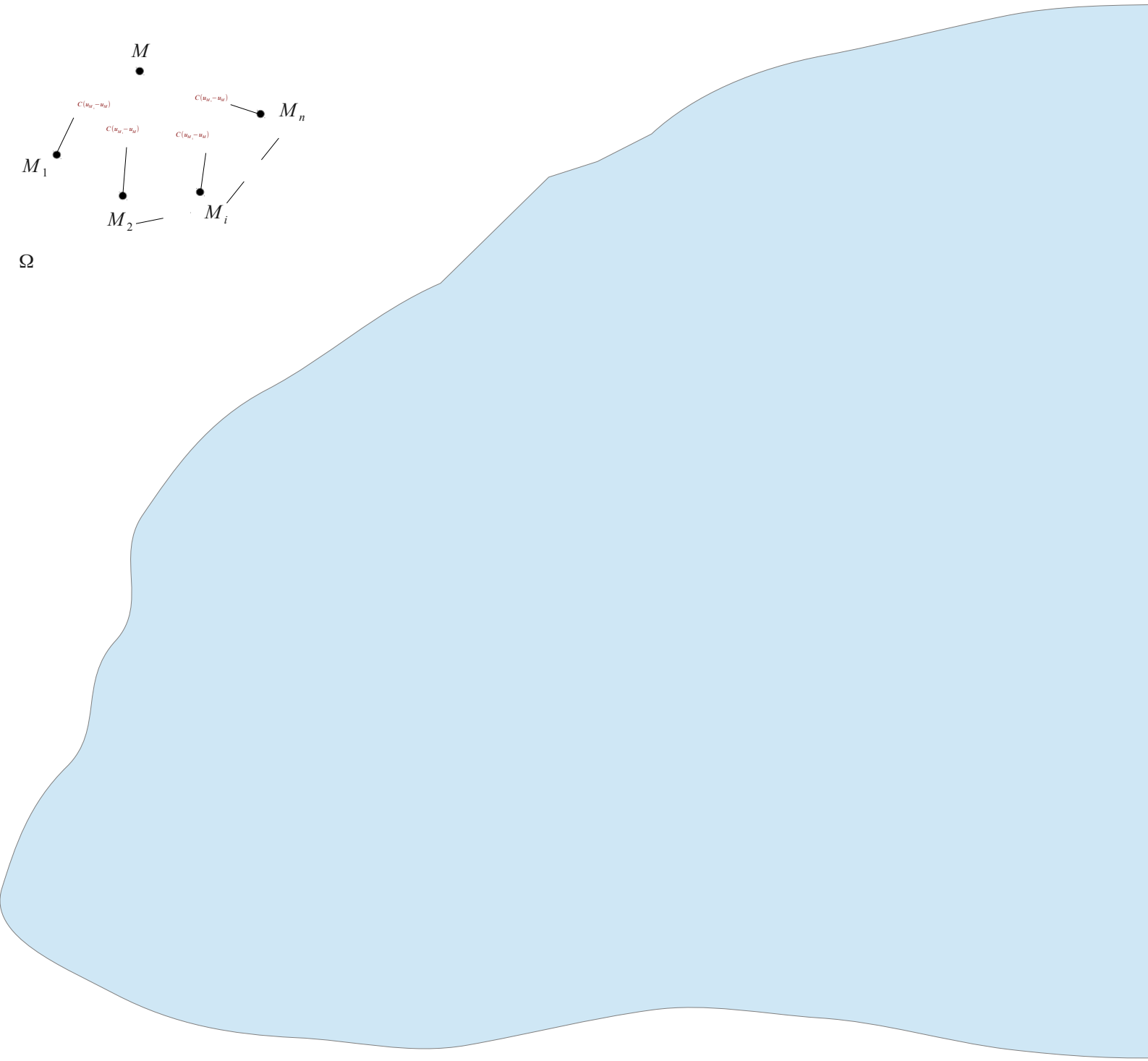

Figure 3.4-1: Example of non-linear relations

This relation is non-linear because it depends on displacements of the various nodes M_i .

3.4.1 Problem of balance under nonlinear conditions of equalities

One supposes the existence of a discrete non-linear equality $C(u)$ of $\mathbb{R}^n$ in $\mathbb{R}$ depending on the solution $u \in R^n$ such that the following problem is had:

$$\left\{\begin{array}{l}\text{Trouver } u\in V \text{ tel que :}\\ \quad J(u)=\min_{v\in V} J(v)\equiv\{L^{\text{int}}(u,v)-L^{\text{ext}}(u,v)\}\\ \quad \text{Avec : } V=\{v\in R^n \text{ tel que } Bv=0 \text{ et } C(v)=0\}\end{array}\right. \tag{109}$$

It is supposed that $C(.)$ is a differentiable function[3] of class at least one. The preceding problem (107) and the problem (109) are such as one seeks the minimum in an area of acceptable solutions $V\subset R^n$. The difficulty lies in the construction a priori of the whole of the acceptable solutions, which is not direct in the case of the problem (109) because of unknown character (depend on the solution) of this acceptable space. One will use the technique of dualisation by the multipliers of Lagrange, one writes the Lagrangian one increased of this system:

$$L(v,\lambda_l^*,\lambda_{nl}^*)=J(v)+\lambda_l^* Bv+\lambda_{nl}^* C(v) \tag{110}$$

From where the problem following equivalent to the problem (109):

$$\begin{array}{c}\text{Trouver les extrémums locaux } \boldsymbol{u}\in\mathbb{R}^n,\boldsymbol{\lambda_l}\in\mathbb{R} \text{ et } \boldsymbol{\lambda_{nl}}\in\mathbb{R}\\ \text{de } L(v,\lambda_l^*,\lambda_{nl}^*)\\ \forall(v,\lambda_l^*,\lambda_{nl}^*)\in\mathbb{R}^n\times\mathbb{R}\times\mathbb{R}\end{array} \tag{111}$$

For that, it is enough to establish the conditions of stationnarity of Lagrangian, that is to say:

$$\left\{\begin{array}{l}\partial_v L(v,\lambda_l^*,\lambda_{nl}^*)\big|_{u,\lambda_l,\lambda_{nl}}\delta v=0\\ \partial_{\lambda_l^*} L(v,\lambda_l^*,\lambda_{nl}^*)\big|_{u,\lambda_l,\lambda_{nl}}\delta\lambda_l^*=0\\ \partial_{\lambda_{nl}^*} L(v,\lambda_l^*,\lambda_{nl}^*)\big|_{u,\lambda_l,\lambda_{nl}}\delta\lambda_{nl}^*=0\end{array}\right. \quad \forall(\delta v,\delta\lambda_l^*,\delta\lambda_{nl}^*)\in\mathbb{R}^n\times\mathbb{R}\times\mathbb{R} \tag{112}$$

From where the non-linear system following to solve:

$$\left\{\begin{array}{l}L^{\text{int}}(u,\delta v)-L^{\text{ext}}(u,\delta v)+\mathbf{B}^T\lambda_l\delta v+\nabla\mathbf{C}^T\lambda_{nl}\delta v=0\\ \delta\lambda_l^*\mathbf{B}u=0\\ \delta\lambda_{nl}^*\mathbf{C}(u)=0\end{array}\right. \quad \forall(\delta v,\delta\lambda_l^*,\delta\lambda_{nl}^*)\in\mathbb{R}^n\times\mathbb{R}\times\mathbb{R} \tag{113}$$

That one will write in more compact form:

$$S(u,\lambda)=0 \tag{114}$$

3.4.2 Linearization of the problem

To solve this problem one also uses the method of Newton. But the system should be linearized (113). One places oneself at the step of time t_i (by simplification of the writings, one omits to specify the dependence of the quantities to the step of time). One approximates the quantities to the iteration of Newton n, compared to these same quantities with the iteration $n-1$:

$$S(u^n,\lambda^n)\approx S(u^{n-1},\lambda^{n-1})+\langle\partial_u S(u^{n-1},\lambda^{n-1}),\Delta u\rangle+\langle\partial_\lambda S(u^{n-1},\lambda^{n-1}),\Delta\lambda\rangle\approx 0 \tag{115}$$

One poses:

$$\langle K(u^{n-1}),\Delta u\rangle=\langle\partial_u S(u^{n-1},\lambda^{n-1}),\Delta u\rangle+\langle\partial_\lambda S(u^{n-1},\lambda^{n-1}),\Delta\lambda\rangle \tag{116}$$

By developing all the terms:

3 If $C(.)$ then the formalism general is not-differentiable does not change except for the correct definition of the generalized jacobien of the nondifferentiable function (see [R5.03.52] for example).

$$\begin{aligned}\langle K(u^{n-1}),\Delta u\rangle=&\delta v\left\{\partial_u L^{\text{int},n-1}\Delta u-\partial_u L^{\text{ext},n-1}\Delta u+\partial^2_{u^2}\mathbf{C}^{n-1}\lambda_{nl}^{n-1}\Delta u\right\}\\&\delta v\left\{\mathbf{B}^T\Delta\lambda_l^{n-1}\right\}+\delta\lambda_l\left\{\mathbf{B}\Delta u\right\}\\&\delta v\left\{\partial_u\mathbf{C}^{n-1}\Delta\lambda_{nl}^{n-1}\right\}+\delta\lambda_{nl}\left\{\partial_u\mathbf{C}^{n-1}\Delta u\right\}\end{aligned}\tag{117}$$

There is finally the following system:

$$\langle K(u^{n-1}),\Delta u\rangle=\begin{Bmatrix}\delta v & \delta\lambda_l & \delta\lambda_{nl}\end{Bmatrix}\begin{bmatrix}K^{\text{int},n-1}+\lambda_{nl}^{n-1}\nabla\nabla\mathbf{C}^{n-1} & \mathbf{B}^T & \nabla^T\mathbf{C}^{n-1}\\ \mathbf{B} & 0 & 0\\ \nabla\mathbf{C}^{n-1} & 0 & 0\end{bmatrix}\begin{Bmatrix}\Delta u\\ \Delta\lambda_l\\ \Delta\lambda_{nl}\end{Bmatrix}\tag{118}$$

With:

- $K^{\text{int},n-1}=\partial_u L^{\text{int},n-1}$ the classical tangent matrix (see 2.3.2 and 2.4.3);
- $\nabla\mathbf{C}^{n-1}=\partial_u\mathbf{C}^{n-1}$ the matrix jacobienne of the non-linear relation;
- $\nabla\nabla\mathbf{C}^{n-1}\lambda_{nl}^{n-1}=\partial^2_{u^2}\mathbf{C}^{n-1}\lambda_{nl}^{n-1}$ the Hessienne matrix of the nonlinear relation

It is found following approached problem, Trouver increments $\Delta u\in\mathbb{R}^n$, $\Delta\lambda_l\in\mathbb{R}$ and $\Delta\lambda_{nl}\in\mathbb{R}$ system in prediction (linearization around the step of time i). With the §2.3.5, we found the expression of the increment of loading *mechanics* $\Delta\mathbf{L}_i^{\text{méca}}$:

$$\Delta\mathbf{L}_i^{\text{méca}}=\mathbf{L}_i^{\text{méca}}-\mathbf{Q}_{i-1}^T.\boldsymbol{\sigma}_{i-1}\tag{119}$$

For the linear limiting conditions, the paragraph § 3.3.1 in also the expression gave.

$$\begin{bmatrix}K_{i-1}^{\text{int}}+\lambda_{nl,i-1}\nabla\mathbf{C}_{i-1} & \mathbf{B}^T & \nabla^T\mathbf{C}_{i-1}\\ \mathbf{B} & 0 & 0\\ \nabla\mathbf{C}_{i-1} & 0 & 0\end{bmatrix}\begin{Bmatrix}\Delta u\\ \Delta\lambda_l\\ \Delta\lambda_{nl}\end{Bmatrix}=\begin{Bmatrix}\mathbf{L}_i^{\text{méca}}-\mathbf{Q}_{i-1}^T.\boldsymbol{\sigma}_{i-1}-\mathbf{B}^T.\boldsymbol{\lambda}_{i-1}+\Delta\mathbf{L}_i^{\text{varc}}\\ \mathbf{B}u_i\\ \mathbf{C}_i u_i\end{Bmatrix}\tag{120}$$

It is advisable to note the difference enters $\mathbf{B}$, matrix of the linear relations and $\mathbf{C}_i$ matrix of the non-linear relations. Indeed, the matrix $\mathbf{B}$ is constant during all calculation, while the matrix $\mathbf{C}_i$ change with each iteration of Newton. It is for that the latter is subscripted by i, contrary to the matrix $\mathbf{B}$. In an equivalent way, during the iterations of Newton n, one must solve the following system:

$$\begin{bmatrix}K^{\text{int,n-1}}+\lambda_{nl}^{n-1}\nabla\nabla\mathbf{C}^{n-1} & \mathbf{B}^T & \nabla^T\mathbf{C}^{n-1}\\ \mathbf{B} & 0 & 0\\ \nabla\mathbf{C}^{n-1} & 0 & 0\end{bmatrix}\begin{Bmatrix}\delta u^n\\ \delta\lambda_l^n\\ \delta\lambda_{nl}^n\end{Bmatrix}=\begin{Bmatrix}\mathbf{L}^{\text{méca},n-1}-\mathbf{L}^{\text{int},n-1}-\mathbf{B}^T.\boldsymbol{\lambda}^{n-1}\\ \mathbf{u}^d-\mathbf{B}.\mathbf{u}^{n-1}\\ \mathbf{C}^{n-1}u^{n-1}\end{Bmatrix}\tag{121}$$

Note:

- As in the standard case, it is possible to make quasi-Newton by being unaware of the contribution of $\nabla\nabla\mathbf{C}$ with the tangent matrix. But it is a choice of the developer because the user does not have access to the choice of reactualization of this term contrary to the case general;
- The problem becoming non-linear in limiting terms of conditions, it is necessary to rock with a reactualized matrix all the iterations of Newton (`REAC_ITER=1`). A message of alarm warns you if you do not do it;

3.4.3 Adaptation of the convergence criteria

It is important to define well the criterion of stop at the end of each iteration of Newton as well after the prediction as during the correction. One recalls (see §2.5) that in *Code_Aster, one can define it several manners.* One clarifies the adaptation here of `RESI_GLOB_MAXI` and `RESI_GLOB_RELA` with the non-linear cases.

The criterion `RESI_GLOB_MAXI` consist in checking that the infinite standard of the residue is lower than the value γ specified by the user. It is necessary to introduce the contribution of the non-linear limiting conditions:

$$\left\|\mathbf{Q}^T.\boldsymbol{\sigma}_i^n+\mathbf{B}^T.\lambda_i^n+\nabla\mathbf{C}_i^{n,T}.\lambda_{nl,i}^n-\mathbf{L}_i^{\text{méca}}\right\|_\infty\leq\gamma\tag{122}$$

The criterion RESI_GLOB_RELA (selected by default) amounts checking that the residue is sufficiently small, like previously, and this compared to a quantity representative of the loading.

$$\frac{\left\|\mathbf{Q}^{T}.\boldsymbol{\sigma}_{i}^{n}+\mathbf{B}^{T}.\lambda_{i}^{n}+\nabla\mathbf{C}_{i}^{n,T}.\lambda_{nl,i}^{n}-\mathbf{L}_{i}^{\text{méca}}\right\|_{\infty}}{\left\|\mathbf{L}_{i}^{\text{méca}}+\mathbf{L}_{i}^{\text{varc}}+\mathbf{B}^{T}.\lambda_{i}^{n}+\nabla\mathbf{C}_{i}^{n,T}.\lambda_{nl,i}^{n}\right\|_{\infty}}\leq\eta \qquad (123)$$

4 Linear research

Linear research here exposed relates to linear research in the absence of piloting.

4.1 Principle

The introduction of linear research into the operator STAT_NON_LINE result from a report: the method of Newton with consistent matrix does not converge in all the cases, in particular when one leaves too much far from the solution. In addition, the use of matrices other than the consistent tangent matrix can, when they are too "flexible", lead to divergence. Linear research makes it possible to secure such divergences against.

It consists in considering $(\delta \mathbf{u}_i^n, \delta \boldsymbol{\lambda}_i^n)$, either like the increment of displacements and the multipliers of Lagrange, but as a direction of research in which one will seek to minimize a functional calculus (the energy of the structure). A step of advance will be found ρ in this direction, and the actualization of the unknown factors will consist in making:

$$\begin{cases} \mathbf{u}_i^n = \mathbf{u}_i^{n-1} + \rho . \delta \mathbf{u}_i^n \\ \boldsymbol{\lambda}_i^n = \boldsymbol{\lambda}_i^{n-1} + \rho . \delta \boldsymbol{\lambda}_i^n \end{cases} \quad (124)$$

In the absence of linear research (by default) the scalar ρ is of course equal to 1.

4.2 Minimization of a functional calculus

In order to be better convinced of the founded good of linear research, one can interpret the method of Newton as a method of minimization of a functional calculus (if the tangent matrices are symmetrical). We insist on the fact that the equations obtained are rigorously those of the method of Newton exposed in [the §2] and that only the way of reaching that point is different.

"The talk the dualisation of the boundary conditions of Dirichlet and we place forget" to simplify on the assumption of the small deformations. The functional calculus is considered:

$$J : V \to \mathbb{R}$$
$$\mathbf{u} \to J(\mathbf{u}) = \int_\Omega \Phi(\boldsymbol{\varepsilon}(\mathbf{u})) . d\Omega - \int_\Omega \mathbf{f} . \mathbf{u} . d\Omega - \int_\Gamma \mathbf{t} . \mathbf{u} . d\Gamma \quad (125)$$

where density of free energy Φ allows to connect the tensor of the constraints $\boldsymbol{\sigma}$ with the tensor of the linearized deformations $\boldsymbol{\varepsilon}$ by the relation $\boldsymbol{\varepsilon} = \frac{\partial \Phi}{\partial \boldsymbol{\sigma}}$ in the case of the hyperelasticity (one generalizes this situation with the others nonlinearities in the continuation of the document). The functional calculus J being convex, to find the minimum of J is equivalent to cancel its gradient, that is to say:

$$\nabla J(\mathbf{u}) . \mathbf{v} = 0 \quad \forall \mathbf{v} \in V \quad (126)$$

What is exactly the Principle of Virtual Work since:

$$\nabla J(\mathbf{u}) . \mathbf{v} = \int_\Omega \boldsymbol{\sigma}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) . d\Omega - \int_\Omega \mathbf{f} . \mathbf{v} . d\Omega - \int_\Gamma \mathbf{t} . \mathbf{v} . d\Gamma \quad (127)$$

Thus, to solve the equations resulting from the Principle of Virtual Work (bases problem formulated in [the §1.3]) is equivalent to minimize the functional calculus J who represents the energy of the structure (decreased energy internal of the work of the external forces $\mathbf{f}$ and $\mathbf{t}$).

4.3 Method of minimization

Minimization is made in an iterative way, classically in two times with each iteration:

- Calculation of a direction of research δ along which one will seek reiterated according to,

- Calculation of the best step of advance ρ in this direction: $\mathbf{u}^{n+1}=\mathbf{u}^{n}+\rho\,.\,\boldsymbol{\delta}$

In a problem of minimization, the natural idea is to advance in the direction opposed to the gradient of the functional calculus, which is locally the best direction of descent since this direction is normal with the lines of isovaleurs and directed in the direction of the decreasing values Figure 2-4.3-1

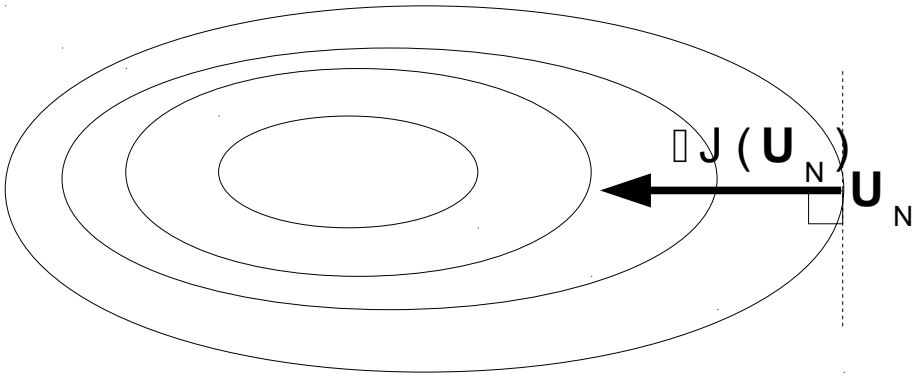

Figure 2-4.3-1

However, it is possible to improve the choice of the direction of descent by using this method of gradient in a metric news. It is what will enable us to find the classical equations of the method of Newton. Let us take the simple example of a problem with two variables x and y for which the functional calculus has the shape of an ellipse whose minimum is in $\left(\frac{\alpha}{a},\frac{\beta}{b}\right)$:

$$J(x,y)=\frac{1}{2}.ax^2+\frac{1}{2}.by^2-\alpha x-\beta y \qquad (128)$$

By choosing like direction of descent the reverse of the gradient of J, one passes from one reiterated to the following (reason on x only) by:

$$x^{n+1}=x^{n}-ax^{n}+\alpha \qquad (129)$$

who does not point towards the solution since the normal in a point of an ellipse does not pass in general by the center of the ellipse

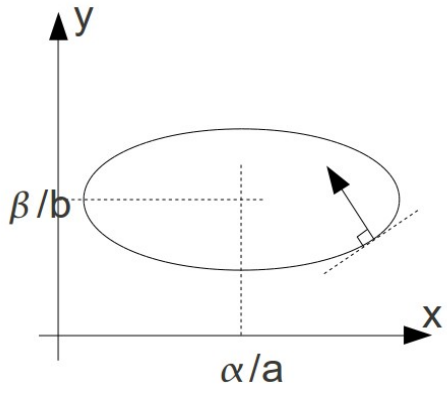

Figure 2 - 4.3-2

On the other hand, if one carries out a change of variables so that the isovaleurs of J become circles:

$$\begin{cases} \bar{x}=\sqrt{a}.x \\ \bar{y}=\sqrt{b}.y \\ \bar{J}(\bar{x},\bar{y})=\frac{1}{2}.(\bar{x}^2+\bar{y}^2)-\frac{\alpha}{\sqrt{a}}.\bar{x}-\frac{\beta}{\sqrt{b}}.\bar{y} \end{cases} \quad (130)$$

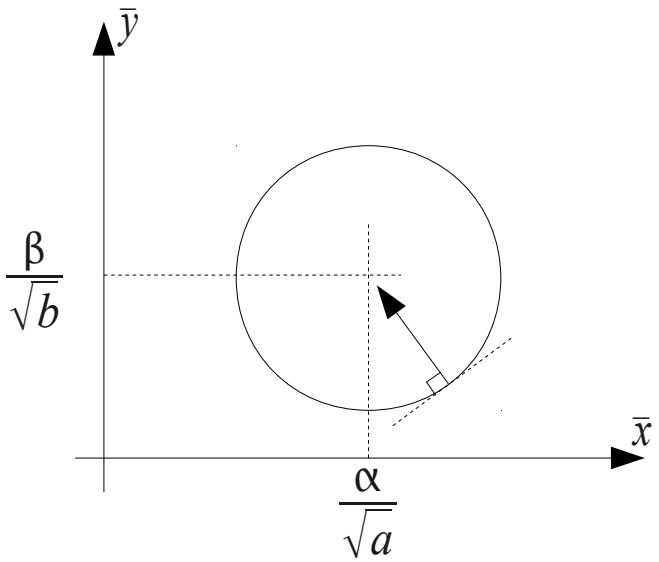

Figure 2-4.3-3

The use of the direction reverses gradient of $\bar{J}$ then allows to obtain the solution in an iteration:

$$\bar{x}^{n+1}=\bar{x}^n-\left(\bar{x}^n-\frac{\alpha}{\sqrt{a}}\right)=\frac{\alpha}{\sqrt{a}}\Rightarrow x^{n+1}=\frac{\alpha}{a} \quad (131)$$

Thus, the use of the method of gradient in the metric news allows an immediate convergence. In a more complicated case (functional calculus convex but different from an ellipse), convergence is not instantaneous but the change of variables makes it possible to appreciably reduce the iteration count necessary.

4.4 Application to the minimization of energy

To simplify, one will place oneself in the discretized linear case where the functional calculus J is worth:

$$J(\mathbf{u})=\frac{1}{2}.\mathbf{u}^T.\mathbf{K}.\mathbf{u}-\mathbf{u}^T.\mathbf{L} \quad (132)$$

One notes $\mathbf{K}$ the matrix of rigidity of the structure, and $\mathbf{L}$ the vector of the imposed loadings. To minimize J, we will use the same method of descent as previously by making a completely similar change of variables as a preliminary. The matrix $\mathbf{K}$ being symmetrical definite positive, its eigenvalues are real positive: one can thus define the “square root” of $\mathbf{K}$ that one will note $\sqrt{\mathbf{K}}$ (also symmetrical). One poses $\bar{\mathbf{u}}=\sqrt{\mathbf{K}}.\mathbf{u}$, the minimization of J is then equivalent to that of:

$$\bar{J}(\bar{\mathbf{u}})=\frac{1}{2}.\bar{\mathbf{u}}^T.\bar{\mathbf{u}}-\bar{\mathbf{u}}^T.\left(\sqrt{\mathbf{K}}\right)^{-T}.\mathbf{L} \quad (133)$$

By using a decomposition by the diagonal:

$$\mathbf{K}=\mathbf{P}.\mathbf{D}.\mathbf{P}^{-1} \quad (134)$$

With $\mathbf{D}$ diagonal, therefore:

$$\sqrt{\mathbf{K}}=\mathbf{P}.\sqrt{\mathbf{D}}.\mathbf{P}^{-1} \tag{135}$$

What leads to:

$$\sqrt{\mathbf{K}^T}.\sqrt{\mathbf{K}}=\mathbf{P}.\sqrt{\mathbf{D}^T}.\sqrt{\mathbf{D}}.\mathbf{P}^{-1}=\mathbf{K} \tag{136}$$

While taking as direction of descent the direction reverses gradient of $\bar{J}$, one obtains:

$$\bar{\mathbf{u}}^{n+1}=\bar{\mathbf{u}}^{n}-\left(\bar{\mathbf{u}}^{n}-\sqrt{\mathbf{K}^{-1}}.\mathbf{L}\right) \tag{137}$$

Maybe, while returning to the initial variables:

$$\mathbf{u}^{n+1}=\mathbf{u}^{n}-\mathbf{K}^{-1}.\left(\mathbf{K}.\mathbf{u}^{n}-\mathbf{L}\right) \tag{138}$$

Or:

$$\mathbf{K}.\left(\mathbf{u}^{n+1}-\mathbf{u}^{n}\right)=\mathbf{L}-\mathbf{K}.\mathbf{u}^{n} \tag{139}$$

One finds the equations of the method of Newton: the matrix $\mathbf{K}$ is Hessienne of the functional calculus J (matrix of the derivative second) and the second member is the difference of the loading and the internal forces, also called residue of balance. Thus method of Newton perhaps interpreted like resulting from the minimization of the energy of the structure via a method of gradient applied after a change of metric.

4.5 Determination of the step of advance

Let us return to the real problem, that of the resolution of $\mathbf{L}_i^{\text{int}}\left(\mathbf{u}_i\right)=\mathbf{L}_i^{\text{ext}}$. This problem can be interpreted like the minimization of the following functional calculus:

$$J=W\left(\mathbf{u}_i\right)-\mathbf{u}_i^T.\mathbf{L}_i^{\text{ext}} \tag{140}$$

where $W\left(\mathbf{u_i}\right)$ corresponds to the discretization, on the basis of the functions of form, the internal energy of the structure:

$$W=\int_\Omega \Phi\left(\boldsymbol{\varepsilon}\left(\mathbf{u}\right)\right).d\,\Omega \tag{141}$$

One calculated by the method of Newton an increment of displacement $\delta\,\mathbf{u}_i^n$ who, in the problem of minimization, is interpreted like a direction of research, according to what precedes. One will calculate the step of advance ρ in this direction allowing to minimize the value of the functional calculus:

$$\underset{\rho\in\mathbb{R}}{\text{Min}}\ \left\{W\left(\mathbf{u}_i^{n-1}+\rho.\delta\,\mathbf{u}_i^n\right)-\mathbf{L}_i^{\text{ext}}\left(\mathbf{u}_i^{n-1}+\rho.\delta\,\mathbf{u}_i^n\right)\right\} \tag{142}$$

To find the minimum of this function scalar of ρ that one will note $f\left(\rho\right)$, one seeks the point where its derivative is cancelled (that amounts making orthogonal the final residue and the direction of research):

$$f'\left(\rho\right)=\left[\delta\,\mathbf{u}_i^n\right]^T.\left[\mathbf{Q}^T.\boldsymbol{\sigma}\left(\mathbf{u}_i^{n-1}+\rho.\delta\,\mathbf{u}_i^n\right)-\mathbf{L}_i^{\text{ext}}\right]=0 \tag{143}$$

$f'\left(\rho\right)$ is the projection of the residue on the direction of research. With the notations of [the §2.2] and by taking of account reactions of support, the scalar equation to solve determine the step of advance ρ , is written:

$$f'\left(\rho\right)=\left[\delta\,\mathbf{u}_i^n\right]^T.\left[\mathbf{Q}^T.\boldsymbol{\sigma}\left(\mathbf{u}_i^{n-1}+\rho.\delta\,\mathbf{u}_i^n\right)+\mathbf{B}^T.\left(\boldsymbol{\lambda}_i^{n-1}+\rho.\delta\,\boldsymbol{\lambda}_i^n\right)-\mathbf{L}_i^{\text{ext}}\right]=0 \tag{144}$$

At the end of linear research, one brings up to date displacements and parameters of Lagrange by:

$$\begin{cases}\mathbf{u}_i^n=\mathbf{u}_i^{n-1}+\rho.\delta\,\mathbf{u}_i^n\\ \boldsymbol{\lambda}_i^n=\boldsymbol{\lambda}_i^{n-1}+\rho.\delta\,\boldsymbol{\lambda}_i^n\end{cases} \tag{145}$$

The test of convergence carries:

- On the maximum number of iterations of linear research indicated by the user under the keyword ITER_LINE_MAXI keyword factor NEWTON (the value by default 0 inhibits linear research, and ρ is worth then 1),
- On the criterion RESI_LINE_RELA given by $f(\rho) \leq \tau . f(0)$, where τ by default 0.1 is worth.

Linear research is to some extent a “insurance” making it possible to guard itself against serious divergences of the method of Newton. When direction of research is “bad” (if the tangent matrix is too flexible, for example), the linear algorithm of research leads to a low value of ρ , which avoids moving away too much from the solution. It is not necessary to do many iterations in the method of secant (two or three are enough to avoid the catastrophes) because each one is rather expensive (should be recomputed the internal forces) and there is not the ambition to find with each iteration of Newton the value of ρ really optimal.

4.6 Calculation of the linear coefficient of research

There exist two methods to calculate it ρ optimal in linear research.

4.6.1 Secant method (METHODE=' CORDE')

So that determination of ρ is not too expensive, one uses a method of secant of which the maximum number of iterations is fixed by the user. The method of secant can be interpreted as a method of Newton where the derivative at the point running is approached by the direction uniting the point running and the preceding point:

$$\rho^{p+1} = \rho^{p} - \frac{\rho^{p} - \rho^{p-1}}{g^{p} - g^{p-1}} \cdot g^{p} = \frac{\rho^{p-1} \cdot g^{p} - \rho^{p} \cdot g^{p-1}}{g^{p} - g^{p-1}} \quad (146)$$

Where one noted $g^{p} = f'(\rho^{p})$. One leaves $\rho^{0} = 0$ and $\rho^{1} = 1$. The method of secant has an order of convergence of about 1.6. It is represented schematically on Figure 2-4.6.1-1 .

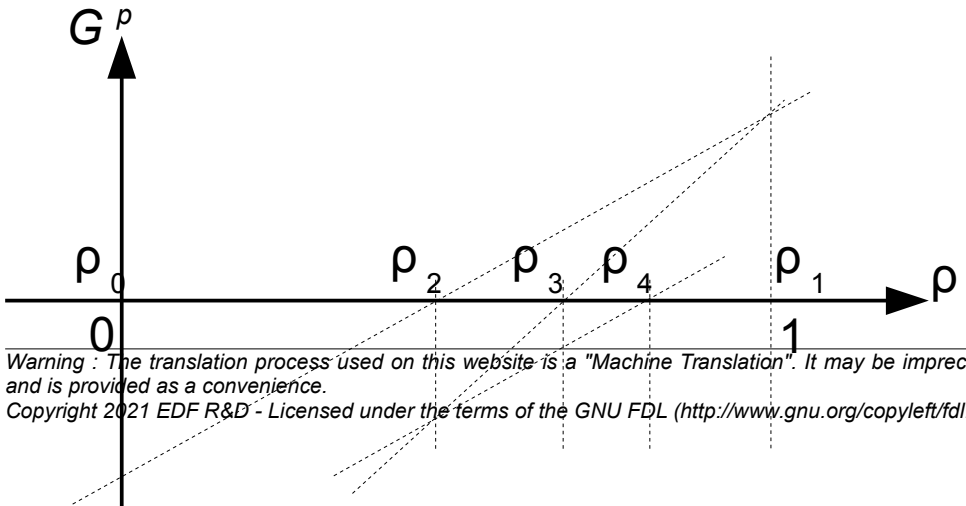

Figure 2-4.6.1-1

4.6.2 Mixed method (METHODE=' MIXTE')

This method mixes several techniques of resolution to be more robust. It consists primarily of the application of a method of the secant (see paragraph the preceding one) between two predetermined terminals. It is by way of the application the method of secant with variable terminals. Here the algorithm used:

1. It is supposed that $f'(0)>0$. If it is not the case, one changes the direction of the direction of descent (while examining ρ negative, which amounts defining f' as being equal to $-f'$
2. One is sought $\rho_{\max}$ positive such as $f'(\rho_{\max})<0$. The method is simply iterative while making $\rho_{n+1}=3.\rho_n$ with $\rho_0=1$ (stage of bracketage or framing)
3. There are thus the two new terminals between which the function changes sign. If it is supposed that the function f' is continuous, it thus exists a solution between these terminals.
4. One applies the method of the secant to this interval: one leaves $\rho^0=0$ and $\rho^1=\rho_{max}$.

4.6.3 Typical case: method of Newton-Krylov

It was specified higher than linear research is carried out simultaneously on the unknown factors $\mathbf{u}$ and $\boldsymbol{\lambda}$ like the formula shows it (Error: Reference source not found) of actualization of the variables. However the functional calculus to be minimized does not present minimum according to the incon Nues $(\mathbf{u},\boldsymbol{\lambda})$, it is indeed about Lagrangian which presents a point saddles, i.e. a minimum in $\mathbf{u}$ and a maximum in $\boldsymbol{\lambda}$ (see [R3.03.01]). This manner of making is thus not licit in the case general.
However, one can show that if the system in prediction is solved “exactly” (all at least with a numerically satisfactory precision), this approach is licit. It is generally the case in the usual use of *Code_Aster*.
It is on the other hand not the case within the framework of the use of the method of Newton-Krylov, where the linear systems are precisely solved in a voluntarily inaccurate way. In this situation, to circumvent the problem, only the unknown factors $\mathbf{u}$ are affected by linear research and the formula of update of the variables thus becomes:

$$\begin{cases}\mathbf{u}_i^n=\mathbf{u}_i^{n-1}+\rho.\delta\mathbf{u}_i^n\\ \boldsymbol{\lambda}_i^n=\boldsymbol{\lambda}_i^{n-1}+\delta\boldsymbol{\lambda}_i^n\end{cases} \quad (147)$$

Insofar as the functional calculus to be minimized has a minimum well in $\mathbf{u}$, the linear procedure of research is licit.

5 Piloting

One will refer to documentation [R5.03.80].

6 Bibliography

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7 History of the versions of the document

Version Aster	Author (S) or contributor (S), organization	Description of the modifications
5	NR. Tardieu, I. Vautier, E. Lorentz EDF R & D MN	
7.4	P.Badel, J.Laverne, NR. Tardieu EDF R & D AMA	
8.5	M.Abbas EDF R & D AMA	Update of the notations, addition of the variables of order.
9.2	M.Abbas EDF R & D AMA	Update of the § 2.2.
9.4	M.Abbas, D.Markovic EDF R & D AMA	Addition of the matrix tangent-secant and mixed linear research.
10.1	M.Abbas EDF R & D AMA	Update of the paragraph on the great deformations.
11.1	NR. Tardieu EDF R & D AMA	Addition of the method of Newton-Krylov.
11.3	Mr. David EDF R & D AMA	Precise details concerning criterion RESI_REFE_RELA