

Assessment of energy into thermomechanical

Summary:

One presents in this documentation the writing of the assessment of energy for a calculation with *Code_Aster*. The calculation of the assessment of energy can be activated in the operators `STAT_NON_LINE` [U4.51.03], `DYNA_NON_LINE` [U4.53.01] and `DYNA_VIBRA` [U4.53.03] on physical basis thanks to the option `ENERGIE=_F` (`()`). This functionality thus covers calculations thermo-hydro-mechanics into quasi-static and dynamics. Are excluded thermal calculations (operators `THER_LINEAIRE`, `THER_NON_LINE` and `THER_NON_LINE_MO`) and modal calculations (operator `DYNA_VIBRA` on modal basis).

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1 Calculation of Bilan of energy of a calculation

The assessment of energy of a calculation can be very useful information. On the one hand, it makes it possible to carry a critical glance on the quality of the results, as well as a residue of balance in the algorithm of Newton. In addition, it informs about the concerned physical phenomena and gives answers to the following questions: which is the energy transmitted to my system? What does it become?

With this intention, one establishes in what follows the writing of the assessment of energy for a calculation with *Code_Aster* on the complete model. We distinguish nature from each term of energy and we attach to define his source.

1.1 Work of a force

Let us consider the evolution at various moments t_i of a deformable solid subjected to a variable external force $\mathbf{F}(t)$. That is to say \mathbf{U}_i the field of solution displacement for each moment t_i and $\mathbf{F}_i = \mathbf{F}(t_i)$. The curve of the effort external according to displacement is given E on Figure 1.1-1. From the energy point of view, the increment of provided work external with the system between two consecutive moments (t_0, t_1) represent the surface under the curve, which is calculated by the method of the trapezoids:

$$A_1 = \int_{t_0}^{t_1} \mathbf{F}(t) \cdot \dot{\mathbf{U}}(t) dt = \frac{\mathbf{F}_0 + \mathbf{F}_1}{2} \cdot (\mathbf{U}_1 - \mathbf{U}_0) = \bar{\mathbf{F}}_1 \cdot \Delta \mathbf{U}_1 \quad (1)$$

where:

- $\bar{\mathbf{F}}_1$ represent the average force on the increment of time (the index is selected as being that of the time of end),
- $\Delta \mathbf{U}_1$ represent the increment of displacement enters t_0 and t_1 .

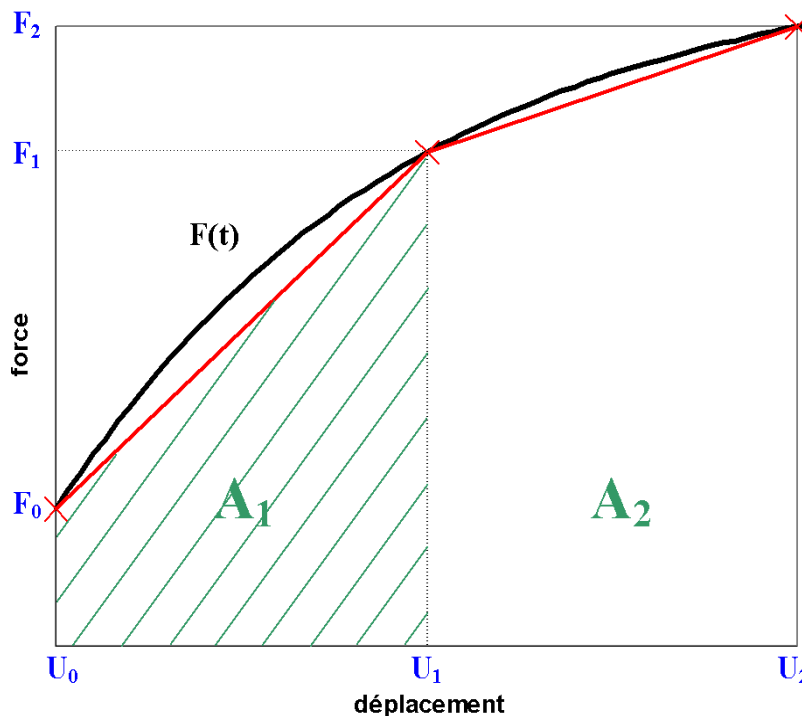


Figure 1.1-1: Curve effort - displacement.

The increment of work of an unspecified force can thus be regarded as the scalar product of two vectors: the average force on the step of time and the increment of displacement.

This method of the calculation of the increment of work of a force is practical within the framework of the digital simulation, since the solution is known at various moments only, corresponding to the selected temporal discretization.

1.2 Assessment of energy

Let us consider the dynamic equilibrium equation of a system in its form discretized in space:

$$\mathbf{M}\ddot{\mathbf{U}}(t) + \mathbf{C}(t)\dot{\mathbf{U}}(t) + \mathbf{R}(\mathbf{U}(t), \dot{\mathbf{U}}(t), t) = \mathbf{L}(t) \quad (2)$$

where:

- \mathbf{U} , $\dot{\mathbf{U}}$ and $\ddot{\mathbf{U}}$ are the vectors of displacements, speeds and accelerations with the nodes,
- \mathbf{M} and \mathbf{C} are the matrices of mass and of damping,
- \mathbf{R} represent the internal forces (in linear elasticity, it acts of the term $\mathbf{K}\mathbf{U}$), which one removed what is regarded as L be forces of damping,
- \mathbf{L} is the vector of the external efforts.

This writing, inspired by [R5.05.05], is simplified here compared to the original writing which utilizes multipliers of Lagrange for the boundary conditions of Dirichlet and the conditions unilateral. Let us note that the matrix of damping $\mathbf{C}(t)$ can depend on time if its construction is based on matrix of the tangent and not elastic stiffness (option AMOR_RAYL_RIGI in the operator DYNA_NON_LINE).

Each term of the equation (2) is homogeneous with a force. Energy evolution of the system between two consecutive moments of calculation t_0 and t_1 results directly in the work of each one of these forces. By taking again the notations of average size and increment of size used in the equation (1), one obtains:

- kinetic increment of energy:

$$\Delta E_{cin} = \int_{\mathbf{U}_0}^{\mathbf{U}_1} (\mathbf{M}\ddot{\mathbf{U}})^T d\mathbf{U} = \int_{t_0}^{t_1} (\mathbf{M}\ddot{\mathbf{U}})^T \dot{\mathbf{U}} dt = \left[\frac{1}{2} \dot{\mathbf{U}}^T \mathbf{M} \dot{\mathbf{U}} \right]_{t_0}^{t_1} = \bar{\mathbf{U}}_1^T \mathbf{M} \Delta \dot{\mathbf{U}}_1 \quad (3)$$

One finds an expression identical to the equation (1) while regarding as force $\mathbf{F} = \mathbf{M}\ddot{\mathbf{U}}$, the operator \mathbf{M} being supposed constant.

- the increment of energy dissipated by damping:

$$\Delta W_{amor} = \overline{\mathbf{C}(t)} \dot{\mathbf{U}}_1^T \cdot \Delta \mathbf{U}_1 \quad (4)$$

As the matrix of damping can be dependent on time, the size should be evaluated $\mathbf{C}(t)\dot{\mathbf{U}}$ with t_0 and with t_1 , then to make the average of it. This stage is neglected in Code_Aster, and one calculates in fact the following size:

$$\Delta W_{amor} = \bar{\mathbf{U}}_1^T \mathbf{C}(t_1) \Delta \mathbf{U}_1 \quad (5)$$

The energy dissipated by damping is thus calculated in an approximate way.

- The increment of total deformation energy:

$$\Delta E_{tot} = \bar{\mathbf{R}}_1^T \Delta \mathbf{U}_1 \quad (6)$$

- The increment of work of the external efforts:

$$\Delta W_{ext} = \bar{\mathbf{L}}_1^T \Delta \mathbf{U}_1 \quad (7)$$

In the presence of rubbing contact, a term of extra effort appears in the equilibrium equation, corresponding by the strength of contact. From the energy point of view, its contribution is calculated easily in a way similar to (1), but it can be taken into account in none energies defined above. One thus creates a new energy which represents the energy stored and/or dissipated by the bonding strengths, that we name ΔW_{liai} . The mechanical assessment of energy of the system is written then:

$$\Delta W_{ext} = \Delta E_{cin} + \Delta E_{tot} + \Delta W_{amor} + \Delta W_{liai} \quad (8)$$

On the assumption that the resolution is strictly exact, the term of left is equal to the sum of the terms of right-hand side. In reality, the digital diagram of resolution induced of the variations for various reasons:

- the algorithm of Newton is an iterative algorithm of resolution, whose convergence is detected when the residue of relative balance of the forces is lower than a certain criterion. By definition, the found solution is thus correct except for a tolerance, which inevitably creates a variation of balance in the energy balance. One can then improve the assessment of energy by hardening the convergence criteria, but the precision reached with the by default criterion is generally satisfactory.
- Among the digital diagrams of temporal integration, only some are not dissipative. To modify the values by default of these diagrams, such as the diagram of Newmark, involve a digital dissipation. The user will be able to refer to documentation [R5.05.05] for more information on dissipation of the digital diagrams of temporal integration.

The assessment of energy finds here a first utility of importance: it makes it possible to quantify the energy dissipated by the digital diagram. In calculations of shocks for example, it is current to use dissipative digital diagrams to filter the high frequencies. One thus defines the energy dissipated by the digital diagram:

$$\Delta W_{sch} = \Delta W_{ext} - \Delta E_{cin} - \Delta E_{tot} - \Delta W_{amor} - \Delta W_{liai} \quad (9)$$

1.3 Construction of the various terms of energy

An energy is regarded as the work of a force. Numerically, the calculation of a term of energy first of all consists in building a total vector corresponding to the sum of all the forces whose contribution to the assessment of energy is stored in the same term. There exist many vectors of force in *Code_Aster*, and we define in this part those which feed each term of energy.

1.3.1 Work of the external forces

One defines as external work work:

- of all the forces associated with orders `AFFE_CHAR_MECA` and `AFFE_CHAR_MECA_F`, except for `FORCE_SOL` entered in the work of the bonding strengths,
- forces resulting from calculation by under-structuring (use of macronutrients),
- of all the forces associated with the order `S_AFFE_CHAR_CINE` and `AFFE_CHAR_CINE_F`. In a strict sense term, the order `AFFE_CHAR_CINE` allows to define boundary conditions of imposed displacement, whose work should be entered as a binding energy. For practical reasons, its contribution is added to external work. In general, it is possible to recover the force corresponding to this imposed displacement. Certain cases can nevertheless pose problem, such as for example the CAS-test `ssnp155a` (see § 2.1.2.1).

1.3.2 Work of the bonding strengths

One defines as work of the bonding strengths work:

- forces of contact and friction exits of the order `DEFI_CONTACT`,
- force resulting from the elements of absorbing border,
- force resulting from the option `FORCE_SOL` in the order `WithFFE_CHAR_MECA`.

1.3.3 Work of the forces of damping

One defines as work of the forces of damping work:

- force of damping from the matrix of damping (term $\mathbf{C}\dot{\mathbf{U}}=(\alpha\mathbf{K}+\beta\mathbf{M})\dot{\mathbf{U}}$),
- force of modal damping (keyword `AMOR_MODAL` in the operators of calculation).

1.3.4 Total deformation energy

The total deformation energy gathers all the contributions which require to integrate a law of behavior. That can lead to arbitrary choices. For example, one enters in the total deformation energy the contribution of the elements of joints or the cohesive elements, although it would be more natural to integrate them into the calculation of the bound energy on the connections. In the same way, when one uses laws of behavior to represent the contact with the discrete elements, the contribution is integrated into the total deformation energy whereas it would be more in its place in the bound energy on the connections. The rule is that, when it is about a behavior carried by finite elements defined in the model, then the contribution is added to E_{tot} .

1.4 Taking into account of an initial state

Let us consider the example of a system mass-arises subjected to an initial shock. In *Code_Aster*, the user can simply give an initial acceleration. That corresponds to the following equation:

$$\begin{aligned}m\ddot{u}(t)+ku(t)&=F(t) \\ u &= 0 \\ F &= 0 \\ \ddot{u} &\neq 0\end{aligned}$$

with like initial conditions: (10)

$$\begin{aligned}u(0) &= 0 \\ \dot{u}(0) &= 0 \\ F(0) &= 0 \\ \ddot{u}(0) &\neq 0\end{aligned}$$

It is noted that there is an incompatibility: the user provides an initial state not balanced. In any rigour, the equations of the dynamics being of the second order in time, there can be only one displacement or a speed imposed on the initial moment. If one wishes to impose an initial acceleration, it would be necessary in theory to give the force which balances the equation of the system. The digital diagram does not need any because that does not influence not on the resolution. Nevertheless, that influences the calculation of the energy balance because without this initial force, the assessment is incorrect. Indeed, energy balance on the first step of time is written then:

$$\begin{aligned}W_{ext} &= E_{tot} + E_{cin} \\ W_{ext} &= 0 \\ E_{tot} &> 0 \\ E_{cin} &> 0\end{aligned} \tag{11}$$

It misses the contribution of the external force which corresponds to this initial acceleration. By taking it into account, one obtains a term then W_{ext} not no one.

In the case general, the assessment of energy can be correct only if calculation starts starting from a balanced state. In the absence of initial state, this condition is implicitly met. A special attention must thus be carried to the various possibilities of introducing a nonvirgin initial state.

1.4.1 Case of the recoveries starting from a state calculated as a preliminary

In this part, one is interested of the recoveries starting from a state calculated as a preliminary, namely the use in `ETAT_INIT` keywords:

- `EVOL_NOLI` for `STAT_NON_LINE` and `DYNA_NON_LINE`,
- `RESULT` for `DYNA_VIBRA`.

In order to calculate each term of energy of the equation (8), it is thus necessary to have with the step recovery:

- nodal vectors of displacement, speed and accelerations,
- matrices of mass and damping,
- internal forces resulting from the state of stress,
- vectors of forces \mathbf{F}_{ext} , \mathbf{F}_{amor} and \mathbf{F}_{liai} .

The nodal vectors of displacement, speed and acceleration, as well as the matrix of mass and the forces internal, are always available. The matrix of damping is not in fact not necessary since one uses the equation (5) to evaluate the energy dissipated by damping, where this matrix is evaluated at the moment t_1 . Only the last three vectors of force require a special attention.

Vectors \mathbf{F}_{amor} and \mathbf{F}_{liai} must be filed because it is impossible to recreate them. Thus, when one activates the calculation of the assessment of energy, one automatically activates the filing of two additional nodal fields called `FORC_AMOR` and `FORC_LIAI`. These fields are intended to be read again in the event of recovery for correctly initializing the calculation of the assessment of energy.

Lastly, concerning the vector \mathbf{F}_{ext} external forces, for `STAT_NON_LINE` and `DYNA_NON_LINE`, it is recomputed at the time of recovery t_0 in accordance with the equation (2) of balance of the system:

$$\mathbf{F}_{ext}(t_0) = \mathbf{M}\ddot{\mathbf{U}}(t_0) + \mathbf{C}(t_1)\dot{\mathbf{U}}(t_0) + \mathbf{R}(\mathbf{U}(t_0), \dot{\mathbf{U}}(t_0)) \quad (12)$$

In the case of a calculation with `DYNA_VIBRA` on physical basis, one saves the external force directly `FORC_EXTE`.

1.4.2 Case of a calculation with an explicitly given initial state

The user can have to provide a nonvirgin initial state in the form of a combination of the following fields:

- one field of displacement (keyword `DEPL`)
- one field of speed (keyword `QUICKLY`)
- a field of acceleration (keyword `ACC E`)
- a stress field (keyword `SIGM`)
- a field of internal variables (keyword `VARI`)

The data of the fields of displacement, speed and acceleration is automatically managed like in the case of an initial state resulting from a preceding calculation, using the equation (12). Let us note that the diagrams in time of the operators of dynamics `DYNA_NON_LINE` and `DYNA_VIBRA` are led S to calculate an initial acceleration if the user does not provide any. This case is managed same manner. By way of an example, in the case of the system mass-arises subjected to an initial acceleration, we build the vector \mathbf{F}_{ext} initial according to:

$$\mathbf{F}_{ext}(t_0) = m\ddot{\mathbf{u}}(t_0) \quad (13)$$

The data of a stress field or internal variables is automatically managed also, since these sizes intervene in the calculation of the term $\mathbf{R}(\mathbf{U}(t_0), \dot{\mathbf{U}}(t_0))$ equation (12).

1.4.3 Initial energy state

It is important to note that the assessment of energy is provided in form incremental E . Thus, it is possible to calculate only one variation of the various terms of energy between two moments of calculation. It is besides this information which is useful in order to know the various transfers of energy. When the initial state of one calculation is provided, it is impossible to calculate the initial energy state. Consequently, the various terms of the assessment of energy are always initialized to 0.

2 Assistance with the use and applications

2.1.1 The Councils

In what follows, we indicate some good practices facilitating obtaining a satisfying assessment of energy.

- **To use an adapted formalism**

The whole of calculations presented falls under a Lagrangian configuration. Indeed, one utilizes a term of average effort on the step of time, obtained by summoning a force written with the preceding step with a force written with the current step. That does not pose a problem for the operator `DYNA_VIBRA`. But that can generate an incorrect assessment of energy for `STAT_NON_LINE` and `DYNA_NON_LINE`, when formalism employed definite under the keyword factor `BEHAVIOR` is:

- `PETIT_REAC`
- `SIMO_MIEHE`

In these two cases, it is advised to take small steps of time to limit the difference between the configurations of calculation of a step of time to the other.

- **To start from a balanced state**

A first precaution is to start from a balanced initial state. Balance is ensured by calculating the external force F_{ext} who balances the initial state (see § 1.4.1). In the majority of the cases, that corresponds to reality. It nevertheless is highly advised to start from a state already balanced when that is possible.

- **To use adapted convergence criteria**

Another point important to announce is the influence of the convergence criteria on the quality of the assessment of energy. The convergence of calculation is ensured except for a tolerance, through the value of `RESI_GLOB_RELA` or `RESI_GLOB_MAXI`. When this criterion is too loose, digital dissipation can become considerable. In case of doubt, it is advised to start again calculation with a criterion more tightened, in order to check that the energy dissipated by integration decreases.

- **To prefer the order `AFFE_CHAR_MECA` with the order `AFFE_CHAR_CINE`**

The order `AFFE_CHAR_CINE` is particular. It consists, at the time of the resolution, to remove the degrees of freedom where a displacement is imposed. This functionality is interesting, since it makes it possible to reduce the size of the system to be solved. Nevertheless, it can pose problem in the evaluation of the energy balance under certain conditions, certainly rather rare. An example is given in the part 2.1.2.1.

2.1.2 Some applications

In this part, we choose some CAS-tests to decipher the assessment of energy of it. Calculations are carried out with version 11.1.12 of *Code_Aster*.

2.1.2.1 CAS-test ssnp155a

This test models a stamping of a sheet by a punch in a matrix (figure 2.1.2.1-1). The structure is modelled in plane deformations. One takes account of symmetry to represent only one half. The punch and the die are modelled in elements of edge, on which one imposes a displacement using the order `AFFE_CHAR_CINE`. One then obtains in the end calculation an obviously incorrect assessment of energy, since W_{ext} is null and since W_{sch} compared to the other terms of energy (table should be very weak 2.1.2.1-1).

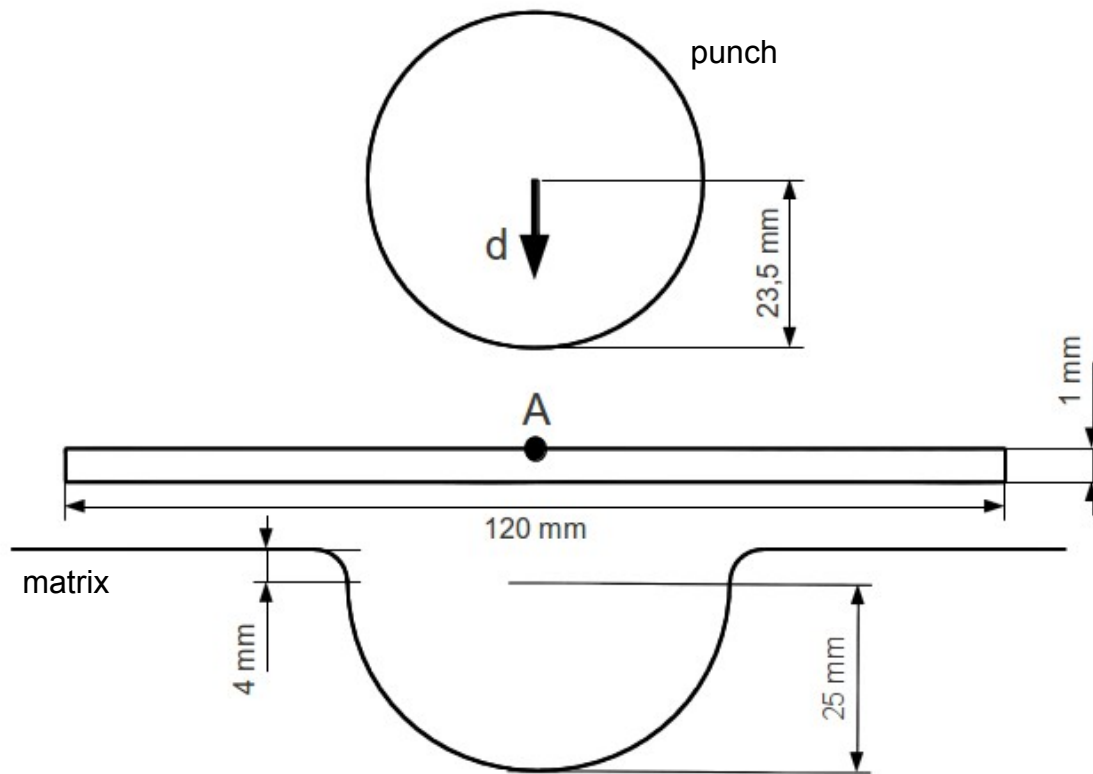


Figure 2.1.2.1-1: Geometry of the CAS-test ssnp155a

W_{ext}	E_{tot}	E_{cin}	W_{liai}	W_{sch}
0	6,8808E+01	3,7883E-05	1,4873E-01	-6,8957E+01

Table 2.1.2.1-1 : Assessment of energy of the CAS-test ssnp155a at the end of the calculation

The explanation is the following one: the fact of using the order `AFFE_CHAR_CINE` remove resolution the unit of the degrees of freedom of the punch. To calculate the contribution to work external of the displacements imposed via the order `AFFE_CHAR_CINE`, one builds the vector of the displacements restricted with the nodes on which a displacement is imposed, and one uses the equation (1) with like the vector of the internal forces. In this CAS-test, external work is only that due to the imposed displacement of the punch. But as it is modelled only with elements of edge, which do not have rigidity, their contribution to the vector of the internal forces is worthless. One is thus in the incapacity to recover the force which corresponds to imposed displacement, and one obtains an external work no one.

To obtain a correct assessment, it is enough to use the order `AFFE_CHAR_MECA` to impose displacement. With this one, in order to guarantee the respect of the conditions of imposed displacement, multipliers of Lagrange are built corresponding in fact to the force to take into account in the calculation of external work. There another solution would have been to net the punch in order to be able to calculate the internal forces. In both cases, one leads then to the assessment of energy indicated in the table 2.1.2.1-2 below:

W_{ext}	E_{tot}	E_{cin}	W_{liai}	W_{sch}
6,8979E+01	6,8808E+01	3,7883E-05	1,4873E-01	2,2804E-02

Table 2.1.2.1-2 : Assessment of energy with use of `AFFE_CHAR_MECA`

The balance of the assessment clearly improved. Nevertheless, the term W_{sch} remain significant. It is by way of with the use of a dissipative diagram HHT. When one uses a diagram of nondissipative Newmark, the term W_{sch} compared to other energies (table becomes negligible 2.1.2.1-3) :

W_{ext}	E_{tot}	E_{cin}	W_{liai}	W_{sch}
6,8947E+01	6,8872E+01	1,6589E-02	5,7774E-02	-1,4257E-08

Table 2.1.2.1-3 : Assessment of energy with use of AFFE_CHAR_MECA and of a nondissipative diagram

2.1.2.2 CAS-test sdlv120a

This CAS-test, illustrated on the figure 2.1.2.2-1 , models an infinite elastic bar in which one creates one compression wave by imposing a displacement on the one of his ends. The other end of the bar is affected of elastic paraxial elements of order 0 intended to apply conditions absorbing to the border of the grid, in order to give an account of the infinite medium.

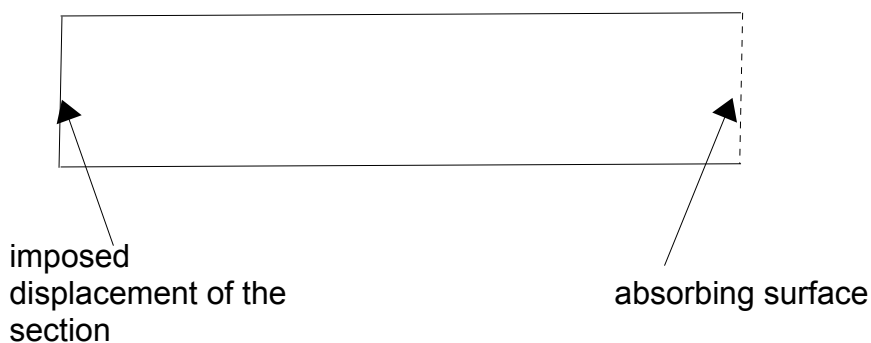


Figure 2.1.2.2-1: Geometry of the CAS-test sdlv120a

One then obtains the following evolution represented on the figure 2.1.2.2-2 for various put energies concerned:

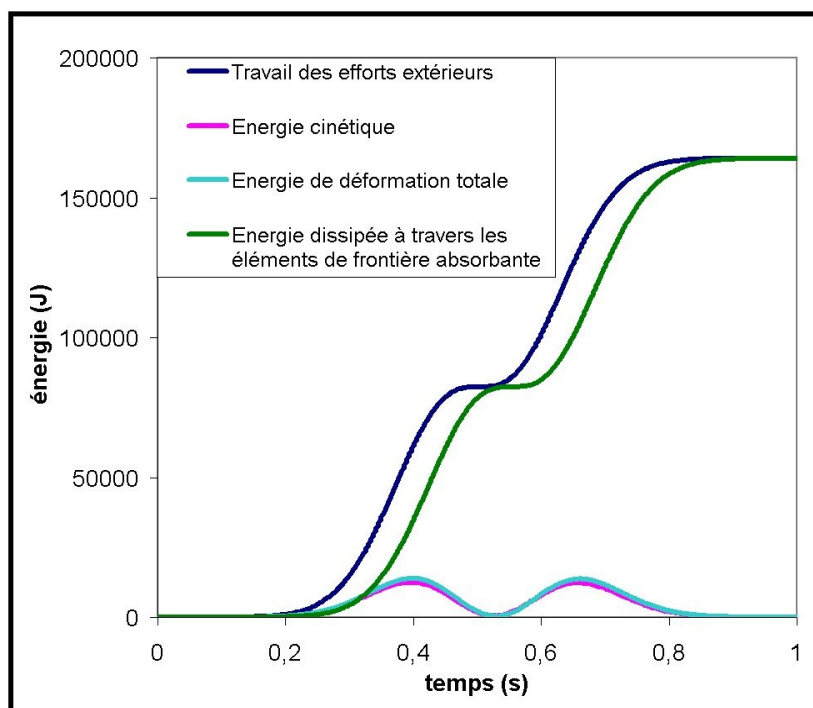


Figure 2.1.2.2-2: Energy evolution in the CAS-test sdlv120a

It is observed that the energy brought by outside is propagated in the bar in the form of total kinetic energy and deformation energy before being quickly dissipated thanks to the elements of absorbing border.

2.1.2.3 CAS-test wtnv109a

This CAS-test models the effect of mechanics and hydraulics on thermics. An element is stretched by imposing a displacement in the direction to him z , while applying a constant water pressure to him, which leads to a reduction in its temperature. We chose it to illustrate the influence of the convergence criteria on the balance of the assessment of energy.

In the table 2.1.2.3-1, one presents the assessment of energy with the value by default of the criterion RESI_GLOB_RELA, namely $1.E-6$, then for a value of $1.E-12$.

RESI_GLOB_RELA	W_{ext}	E_{tot}	W_{sch}
1.E-6	1,1296E+02	1,1303E+02	-7,0833E-02
1.E-12	1,1303E+02	1,1303E+02	-2,3590E-12

Table 2.1.2.3-1: Assessment of energy of the CAS-test wtnv109a

It is noted that the variation of balance, symbolized by the value of W_{sch} , was decreased by a factor 10.

3 History of the versions of the document

Version Aster	Author (S) or contributor (S), organization	Description of the modifications
11.1	L. Idoux EDF R & D AMA	