Assessment of energy in thermo mechanical

Abstract:

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

Contents

1 Computation of the assessment of energy of a computation

the assessment of energy of a computation 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 equilibrium 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 the model follows the writing of the assessment of energy for a computation *with* Code_Aster on complete. 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 times t_i of a deformable solid subjected to a variable external force $\mathbf{F}(t)$. Either $\mathbf{U}_i$ the field of solution displacement for each time t_i and $\mathbf{F}_i=\mathbf{F}(t_i)$. The curve of the external force 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 times (t_0,t_1) represents the area under the curve, which is calculated by the method of the trapezoids:

$$A_1=\int_{t_0}^{t_1}\mathbf{F}(t).\dot{\mathbf{U}}(t)=\frac{\mathbf{F_0}+\mathbf{F_1}}{2}.(\mathbf{U}_1-\mathbf{U}_0)=\bar{\mathbf{F}}_1.\Delta\mathbf{U}_1 \quad (1)$$

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

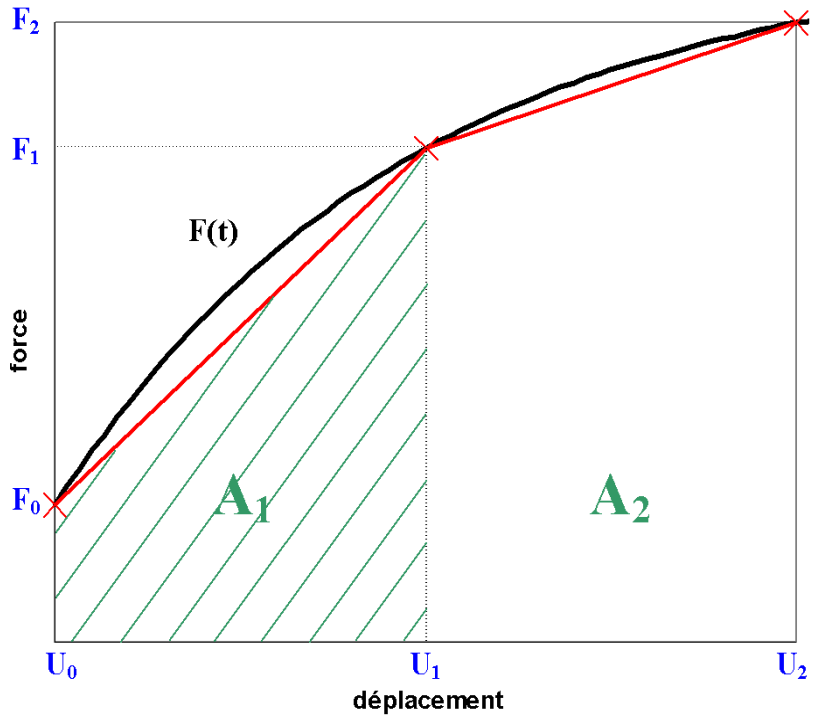


Figure 1.1-1: Curve force - displacement.

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

This method of the computation of the increment of work of a force is practical in the frame of computational simulation, since the solution is known at various times only, corresponding to the selected temporal discretization.

1.2 Assessment of energy

Let us consider the dynamic balance 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 displacements, velocities and accelerations with the nodes,
- $\mathbf{M}$ and $\mathbf{C}$ are the mass matrixes and of damping,
- $\mathbf{R}$ represents the internal forces (in linear elasticity, it is the term $\mathbf{K}\,\mathbf{U}$), which one removed what is regarded as L are damping forces,
- $\mathbf{L}$ is the vector of the external forces.

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

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

- the increment of kinetic energy:

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

One finds a statement 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:

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

As the damping matrix can be dependant on time, it is necessary to evaluate the quantity $\mathbf{C}(\mathbf{t})\dot{\mathbf{U}}$ 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 quantity:

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

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

- The increment of total strain energy:

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

- the increment of work of the external forces:

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

In the presence of rubbing contact, a term of extra effort appears in the balance 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. In reality, the numerical 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 equilibrium 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 equilibrium in the energy balance. One can then improve the assessment of energy by hardening the convergence criterion, but the accuracy reached with the by default criterion is generally satisfactory.
•Among the numerical diagrams of temporal integration, only some are not dissipative. To modify the values by default of these diagrams, such as the diagram of Newmark, involves a numerical dissipation. The user will be able to refer to documentation [R5.05.05] for more information on dissipation of the numerical 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 numerical diagram. In computations of shocks for example, it is current to use dissipative numerical diagrams to filter the high frequencies. One thus defines the energy dissipated by the numerical 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 computation 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 force vectors 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 commands AFFE_CHAR_MECA and AFFE_CHAR_MECA_F, except for FORCE_SOL entered in the work of the bonding strengths,
•the forces resulting from computation by substructuring (use of macro-elements),
•from all the forces associated with the command S AFFE_CHAR_CINE and AFFE_CHAR_CINE_F. In a strict sense term, command AFFE_CHAR_CINE makes it possible 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 ssnp155a benchmark (see § 8).

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 command DEFI_CONTACT ,
•force resulting from the elements of absorbing border,
•the force resulting from option FORCE_SOL in command AFFE_CHAR_MECA.

1.3.3 Work of the damping forces

One defines as work of the damping forces work:

•damping force from the damping matrix (term $\mathbf{C}\dot{\mathbf{U}}=(\alpha\mathbf{K}+\beta\mathbf{M})\dot{\mathbf{U}}$),
•of the damping force modal (key word AMOR_MODAL in the operators of computation).

1.3.4 Total strain energy

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

1.4 Taken into account of an initial state

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

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

with like initial conditions: (10)

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

One notes that there is an incompatibility: the user provides an initial state not balanced. In any rigor, the equations of the dynamics being of the second order in time, there can be only one displacement or a velocity imposed on initial time. 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 numerical diagram does not need any because that does not influence the resolution. Nevertheless, that influences the computation of the energy balance because without this initial force, the assessment is incorrect. Indeed, the energy equilibrium on the first time step is written then:

$$\begin{gathered} W_{ext}=E_{tot}+E_{cin} \\ W_{ext}=0 \\ E_{tot}>0 \\ E_{cin}>0 \end{gathered} \quad (11)$$

It misses the contribution of the external force which corresponds to this initial acceleration. In taking into account, one obtains a term then W_{ext} non-zero.

In the general case, the assessment of energy can be correct only if computation starts 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 from a state calculated as a preliminary

In this part, one is interested of the recoveries from a state calculated as a preliminary, namely the use in ETAT_INIT of the key words:
•EVOL_NOLI for STAT_NON_LINE and DYNA_NON_LINE ,
•RESULTAT 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, velocity and accelerations,
- mass matrixes and of damping,
- internal forces resulting from the stress state,
- of the force vectors $\mathbf{F}_{ext}$, $\mathbf{F}_{amor}$ and $\boldsymbol{F}_{liai}$.

The nodal vectors of displacement, velocity and acceleration, as well as the mass matrix and the internal forces, are always available. The damping matrix 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 time t_1 . Only the last three force vectors require a special attention.

The vectors $\mathbf{F}_{amor}$ and $\mathbf{F}_{liai}$ must be filed because it is impossible to recreate them. Thus, when one activates the computation of the assessment of energy, one automatically activates the archivage 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 computation 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 equilibrium of the system:

$$\mathbf{F}_{ext}(t_0)=\mathbf{M}\ddot{\mathbf{U}}(t_0)+\mathbf{C}(t_1)\dot{\mathbf{U}}(t_0)+\mathbf{R}\left(\mathbf{U}(t_0),\dot{\mathbf{U}}(t_0)\right) \qquad \text{formulate1 212}$$

) a computation with DYNA_VIBRA on physical base, one saves external force FORC_EXTE directly.

1.4.2 Case of a computation with an initial state explicitly given

the user can have to provide a nonvirgin initial state in the form of a combination of the following fields:
- a field of displacement (key word DEPL)
- a velocity field (key word QUICKLY)
- a field of acceleration (key word ACC E)
- a stress field (key word SIGM)
- a field of local variables (key word VARI)

the data of the fields of displacement, velocity and acceleration is automatically managed as in the case of an initial state resulting from a preceding computation, using the equation (12). Let us note that the time schemes 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 way. By way of an example, in the case of the spring-mass system subjected to an initial acceleration, we build the vector F_{ext} initial according to:

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

the data of a stress field or local variables is automatically managed also, since these quantities intervene in the computation of the term $\mathbf{R}\left(\mathbf{U}(t_0),\dot{\mathbf{U}}(t_0)\right)$ 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 times of computation. It is besides this information which is useful in order to know the various transfers of energy. When the initial state of a computation 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 Helps 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 a formalism adapted

all computations presented falls under a Lagrangian configuration. Indeed, one utilizes a term of average force on time step, obtained by adding a force written with the preceding step with a force written with the current step. That does not pose a problem for operator DYNA_VIBRA. But that can generate an incorrect assessment of energy for STAT_NON_LINE and DYNA_NON_LINE , when the formalism employed definite under factor key word the COMP_INCR is:
•PETIT_REAC
•SIMO_MIEHE

In these two cases, it is advised to make the small ones time step to limit the difference between the configurations of computation of time step to the other.

•To start from a state balanced

a first precaution is to start from a balanced initial state. The equilibrium is ensured by calculating the external force F_{ext} which balances the initial state (see § 6). 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 criterion on the quality of the assessment of energy. The convergence of computation is ensured except for a tolerance, through the value of RESI_GLOB_RELA or RESI_GLOB_MAXI. When this criterion is too loose, numerical dissipation can become considerable. In case of doubt, it is advised to start again computation with a criterion more tightened, in order to check that the energy dissipated by integration decreases.

•To prefer command AFFE_CHAR_MECA with command AFFE_CHAR_CINE

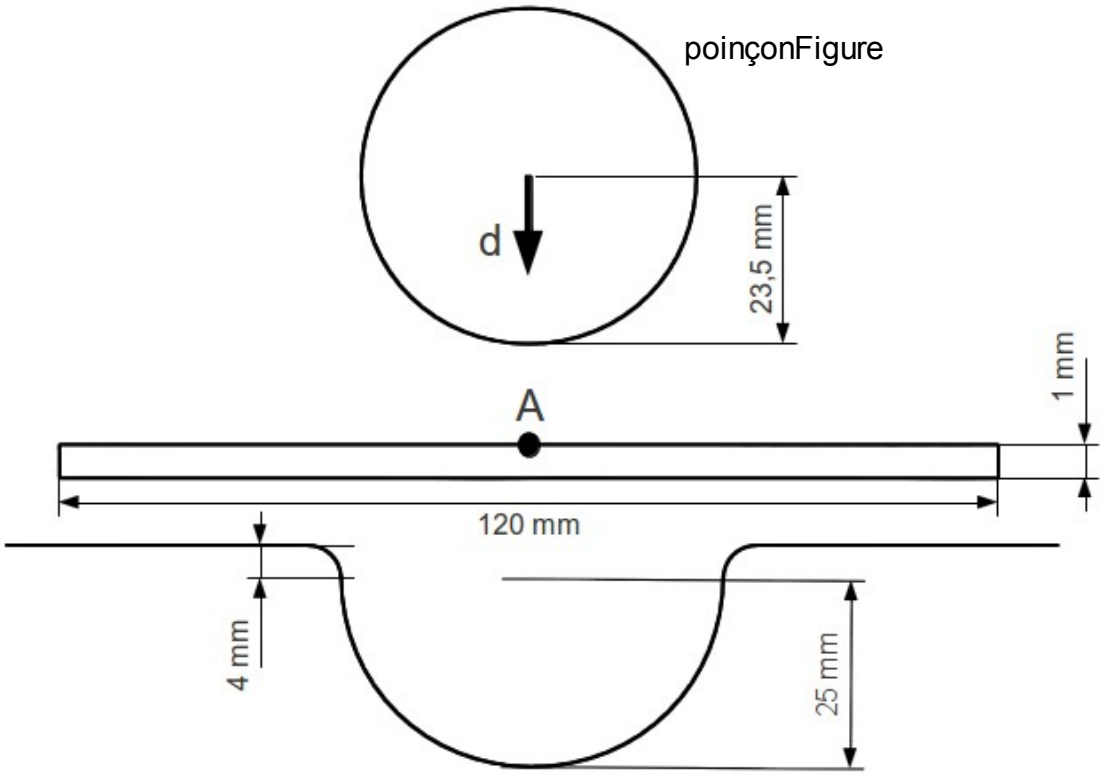
command AFFE_CHAR_CINE is particular. It consists in, during the resolution, removing the degrees of freedom where a displacement is imposed. This functionality is interesting, since it makes it possible to reduce the size of the system to be solved. Nevertheless, it can pose problem in the evaluating of the energy balance under certain conditions, certainly rather rare. An example is given in the 2.1.2.1 8.

2.1.2 Some applications

In this part, we choose some benchmarks to decipher the assessment of energy of it. Computations are carried out with version 11.1.12 of *Code_Aster*.

2.1.2.1 Benchmark ssnp155a

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



2.1.2.1-1: Geometry of the ssnp155amatrice benchmark

W_{ext}	E_{tot}	E_{cin}	W_{liai}	W_{sch}
06,8808E+013,7883E-051,4873E-01-6,8957E+01Tableau				

2.1.2.1-1 : Assessment of energy of the ssnp155a benchmark at the end of the computation

the explanation is the following one: the fact of using command AFFE_CHAR_CINE removes resolution all of the degrees of freedom of the punch. To compute: the contribution to work external of the displacements imposed via command 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 forces the vector of the internal forces. In this case, external work is only that due to the imposed displacement of the punch. But as it is modelled only with edge elements, which do not have a stiffness, their contribution to the vector of the internal forces is null. 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 command AFFE_CHAR_MECA to impose displacement. With this one, in order to guarantee the respect of the conditions of imposed displacement, Lagrange multipliers are built corresponding makes some with the force take into account in the computation 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 2.1.2.1 2.1.2.1-2 below:

W_{ext}	E_{tot}	E_{cin}	W_{liai}	W_{sch}
6,8979E+016,8808E+013,7883E-051,4873E-012,2804E-02Tableau				

2.1.2.1-2 : Assessment of energy with use of AFFE_CHAR_MECA

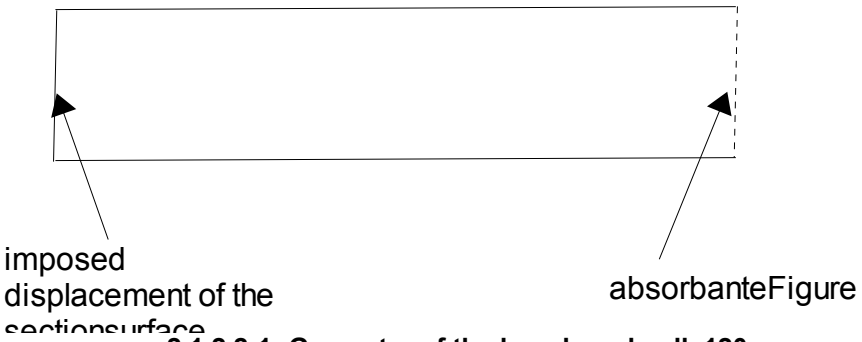
the equilibrium of the assessment clearly improved. Nevertheless, the term W_{sch} significant rest. It is by way of with the use of a dissipative diagram HHT. When one uses a diagram of nondissipative Newmark, the formula W_{sch} becomes negligible compared to other energies (2.1.2.1 2.1.2.1-3):

W_{ext}	E_{tot}	E_{cin}	W_{liai}	W_{sch}
6,8947E+016,8872E+011,6589E-025,7774E-02-1,4257E-08Tableau				

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

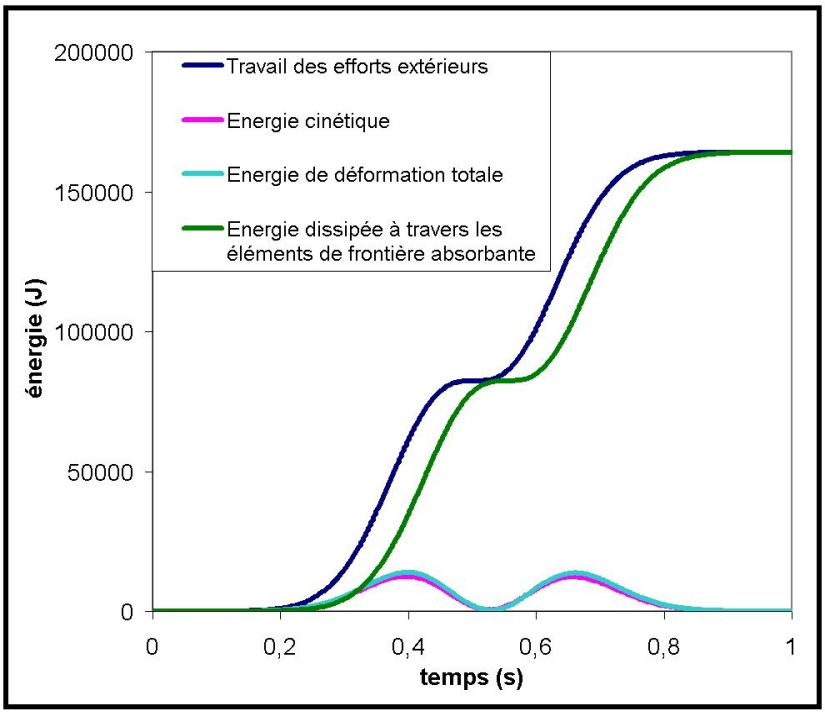
2.1.2.2 sdlv120a Benchmark

This benchmark, illustrated on the 2.1.2.2 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 mesh, in order to give an account of the infinite medium.



2.1.2.2-1: Geometry of the benchmark sdlv120a

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



Appear 2.1.2.2-2: Energy evolution in the benchmark sdlv120a

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

2.1.2.3 Benchmark wtnv109a

This benchmark models the effect of the mechanics and the hydraulics on the thermal. 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 criterion on the equilibrium of the assessment of energy.

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

RESI_GLOB_RELAformule	W_{ext}	E_{tot}	W_{sch}
1.E-61,1296E+021,1303E+02-7,0833E-021.E-121,1303E+021,1303E+02-2,3590E-12Tableau			

2.1.2.3-1: Assessment of energy of the benchmark wtnv109a

One notes that the variation of equilibrium, 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	