

Nonlinear thermics in pointer

Summary

One presents the formulation and the algorithm of the problem of convection-diffusion in stationary nonlinear thermics introduced within the order `THER_NON_LINE_MO` [U4.33.04].

The goal is to solve the equation of heat in a mobile reference frame related to a loading and moving in a given direction and at a speed.

Nonthe linearities of the problems come as well from the characteristics of material which depend on the temperature, as boundary conditions of type radiation.

The problems of this type can be treated with models using of the finite elements of structure plans, axisymmetric and three-dimensional.

Contents

Contents

1	Presentation of the problem.....	3
2	Boundary conditions. Problem of reference to be solved.....	5
3	Variational formulation of the problem.....	6
4	Treatments of nonthe linearities.....	7
4.1	Treatment of nonthe linearity related to the enthalpy.....	7
4.2	Treatment of nonthe linearities related on the nonlinear condition of Fourier and thermal conductivity.....	8
5	Algorithm established in Code_Aster.....	8
6	Principal options of calculation in Code_Aster.....	11
7	Bibliography.....	12
8	Description of the versions of the document.....	12

1 Presentation of the problem

The equation of heat has strong not linearities under certain conditions. It is the case when the material undergoes phase shifts: those are accompanied by an abrupt variation of the characteristic sizes (heat-storage capacity, enthalpy). This nonlinearity is all the more accentuated when with the problem of convection-diffusion is dealt, where appears the term of transport depend on the function enthalpy. The goal of this modeling is to deal with this last problem in permanent mode (stationary case).

In all the cases, it is supposed that the field speed is known a priori. The case of a mobile solid is rather frequent in practice. It relates to in particular the applications of welding or the surface treatment which bring into play a source of heat moving in a given direction and at a speed. The problem of thermics is then studied in a reference frame related to the source.

The problem with the derivative partial results from the equation of the total heat balance on any field Ω who is written:

$$\frac{d}{dt} \int_{\Omega} \rho \beta d \Omega = \int_{\Omega} Q d \Omega - \int_{\partial \Omega} \mathbf{q} \cdot \mathbf{n} d \Gamma \quad \text{éq 1-1}$$

accumulation création + entrée-sortie

In this equation, Ω represent a related, interior field with the studied system, which one follows in his movement, β represent the specific enthalpy of material and ρ indicate its density. Q is a voluminal source of heat, \mathbf{q} is the heat flow through the border $\partial \Omega$ (\mathbf{n} being the external normal), and d/dt is **particulate derivative**.

The first term of [éq 1-1] is written (see for example [bib1]):

$$\frac{d}{dt} \int_{\Omega} \rho \beta d \Omega = \int_{\Omega} \left(\frac{\partial (\rho \beta)}{\partial t} + \text{div}(\rho \beta \mathbf{V}) \right) d \Omega \quad \text{éq 1-2}$$

or, taking into account the conservation of mass $\left(\frac{\partial \rho}{\partial t} + \text{div}(\rho \mathbf{V}) = 0 \right)$ [bib1]:

$$\frac{d}{dt} \int_{\Omega} \rho \beta d \Omega = \int_{\Omega} \left(\rho \frac{\partial \beta}{\partial t} + \rho \mathbf{V} \cdot \text{grad} \beta \right) d \Omega \quad \text{éq 1-3}$$

where \mathbf{V} is the Flight Path Vector of displacement of the field Ω . \mathbf{V} is well informed under the simple keyword CONVECTION orders AFFE_CHAR_THER and AFFE_CHAR_THER_F.

The second term of the second member of [éq 1-1] is written, taking into account the theorem of the divergence and the Fourier analysis ($\mathbf{q} = -k(T)\mathbf{grad} T$) :

$$\int_{\partial\Omega} \mathbf{q} \cdot \mathbf{n} d\Gamma = \int_{\Omega} \text{div} \mathbf{q} d\Omega = - \int_{\Omega} \text{div}(k(T)\mathbf{grad} T) d\Omega \quad \text{éq 1-4}$$

where T is the temperature and $k(T)$ is the thermal conductivity of material, function of the temperature.

The equation [éq 1-1] in front of being satisfied for any field Ω , it comes then:

$$\rho \frac{\partial \beta}{\partial t} + \rho \mathbf{V} \cdot \mathbf{grad} \beta - \text{div}(k(T)\mathbf{grad} T) = Q \text{ in } \Omega \quad \text{éq 1-5}$$

Note:

Let us note that the classical case with, $k(T) = k$ (constant) and $\mathbf{V} = 0$, and where the specific enthalpy is a linear function of the temperature, $\beta(T) = CT$ give again the well-known classical equation:

$$\rho C \frac{\partial T}{\partial t} - k\Delta T = Q \text{ in } \Omega$$

where Δ is the Laplacian and C (constant) the specific heat represents.

The problem with the derivative partial treaty by the order THER_NON_LINE_MO [U4.33.04], consists in solving the equation [éq 1-5] in the stationary case (directly at the permanent state) with boundary conditions on the border $\partial\Omega$.

This problem is formally written in the following form:

$$\begin{aligned} \mathbf{V} \cdot \mathbf{grad} u(T) - \text{div}(k(T)\mathbf{grad} T) = Q, & \quad \text{dans } \Omega, \\ + \text{conditions aux limites} & \quad \text{sur } \partial\Omega \end{aligned} \quad \text{éq 1-6}$$

where we adopted the notation, valid for all the continuation, $u(T) = \rho \beta(T)$ where ρ is constant, defining the voluminal enthalpy.

2 Boundary conditions. Problem of reference to be solved

One will refer, for example, with [R5.02.01] for more information on the boundary conditions thermal of type Dirichlet, Neumann and linear Fourier, and with [R5.02.02] for the boundary conditions of type nonlinear normal flow (nonlinear Fourier).

In enthalpic formulation, the problem of thermics **stationary** thus consist in solving in a field Ω of border on $\partial\Omega$.

$$V \cdot \text{grad } u(T) - \text{div}(k(T) \text{grad } T) = Q \text{ in } \Omega \quad \text{éq 2-1}$$

$$\text{with } k(T) \frac{\partial T}{\partial \mathbf{n}} = \gamma(T_{\text{ext}} - T) \text{ on } \partial_1 \Omega \quad \text{éq 2-2}$$

$$k(T) \frac{\partial T}{\partial \mathbf{n}} = q_0 \text{ on } \partial_2 \Omega \quad \text{éq 2-3}$$

$$k(T) \frac{\partial T}{\partial \mathbf{n}} = \alpha(T) \text{ on } \partial_3 \Omega \quad \text{éq 2-4}$$

$$T = T_0 \text{ on } \partial_4 \Omega \quad \text{éq 2-5}$$

where:

- T_0 : is the temperature imposed on $\partial_4 \Omega$;
- q_0 : is the normal flow imposed on $\partial_2 \Omega$;
- γ : is the coefficient of heat exchange ;
- T_{ext} : is the outside temperature ;
- $\alpha(T)$: is the normal flow of nonlinear type Fourier (radiation).

The equations [éq 2-2], [éq 2-5] the boundary conditions of the types represent, respectively: Linear Fourier, Neumann, nonlinear Fourier and Dirichlet.

The problem of reference [éq 2-1], [éq 2-5] is strongly nonlinear because of nonthe linearities on $k(T)$, $u(T)$ (phase shift) and $\alpha(T)$ (radiation).

3 Variational formulation of the problem

That is to say Ω open of \mathbf{R}^3 , of border $\partial\Omega = \partial_1\Omega \cup \partial_2\Omega \cup \partial_3\Omega \cup \partial_4\Omega$ such as,
for $i \neq j$ and $i, j = 1, \dots, 4$, one a: $\partial_i\Omega \cap \partial_j\Omega = \emptyset$.

That is to say still ψ a sufficiently regular function which is cancelled on $\partial_4\Omega$:
 $\psi \in V = \left\{ y \text{ régulière et } \psi|_{\partial_4\Omega} = 0 \right\}$.

Let us multiply by ψ the two members of the equation [éq 2-1], then let us integrate on Ω . An integration by parts gives then:

$$\begin{aligned} \int_{\Omega} Q y d\Omega &= \int_{\Omega} V \cdot \mathbf{grad} u(T) y d\Omega - \int_{\Omega} \text{div}(k(T) \mathbf{grad} T) y d\Omega \\ &= \int_{\Omega} V \cdot \mathbf{grad} u(T) y d\Omega + \int_{\Omega} k(T) \mathbf{grad} T \cdot \mathbf{grad} y d\Omega - \int_{\partial\Omega - \partial_4\Omega} \left(k(T) \frac{\partial T}{\partial n} y \right) dG \end{aligned}$$

éq 3-1

since ψ is null on $\partial_4\Omega$.

From where, by taking account of the boundary conditions [éq 2-2], [éq 2-3] and [éq 2-4], the variational formulation of the problem of reference which is given by the following equation:

$\forall \psi \in V$

$$\begin{aligned} \int_{\Omega} k(T) \mathbf{grad} T \cdot \mathbf{grad} y d\Omega &+ \int_{\Omega} V \cdot \mathbf{grad} u(T) y d\Omega + \int_{\partial_1\Omega} g T y dG - \int_{\partial_3\Omega} \alpha(T) y dG \\ &= \int_{\Omega} Q y d\Omega + \int_{\partial_1\Omega} \gamma T_{ext} y dG + \int_{\partial_2\Omega} q_0 y d\Omega, \end{aligned} \quad \text{éq 3-2}$$

4 Treatments of nonthe linearities

For the digital resolution of the nonlinear problem that we consider, it is necessary to treat all nonthe linearities.

In our case, let us quote the strong not linearity related to the function enthalpy $u(T)$ who takes into account the solid-liquid phase shift, as well as nonthe linearity related to the possible presence of a boundary condition of nonlinear normal flow (radiation).

Let us recall that in the classical case of the problems of transitory thermics nonlinear without convection, that is to say $V=0$, several methods of resolution are proposed in the literature. There as well exist methods using of the enthalpic formulations as methods using of the formulations in temperature, all having for goal as well as possible to treat to it not linearity related to the enthalpy (phase shift).

We return the reader to the reference [bib5] for a summary of the principal methods met in the literature. However, let us note that because of the difficulty related to the presence of the term of transport $V \cdot \text{grad } u(T)$ in the problem, none of these methods will be employed in the continuation.

As in any iterative process, the goal of the digital diagram in sight is to find a field of temperature T^{n+1} with the iteration $n+1$, starting from the field of temperature T^n , solution of the preceding iteration.

4.1 Treatment of nonthe linearity related to the enthalpy

In order to treat this nonlinearity, the strategy employed in this study was inspired by a technique of resolution of the free problems of borders [bib3], which, in the beginning was proposed in [bib4].

Let us consider the function enthalpy $u(T)$ as being given in a reciprocal form: Temperature function of the enthalpy (opposite of the function $u(T)$). In other terms one will have to treat the relation following Temperature-enthalpy:

$$T = \tau(u) \quad \text{éq 4.1-1}$$

The reason of this choice will be clearer in what follows. Indeed we will have to deal with a problem with two fields: a field of temperature and a field enthalpy. The discretization of the opposite function [éq 4.1-1] makes it possible to as follows increment the field enthalpy according to the current field of temperature (and not the reverse):

The development with the first order of the function $\tau(u)$ is the following,

$$T^{n+1} = \tau(u^n) + \tau'(u^n)(u^{n+1} - u^n), \quad \text{éq 4.1-2}$$

where τ' is the derivative of the function defined by [éq 4.1-1] compared to its argument.

In order to take into account this nonlinearity, and from [éq 4.1-2], one replaces u^{n+1} by an approximation according to the unknown field of temperature T^{n+1} in the following way:

$$u^{n+1} - u^n = \omega(T^{n+1} - \tau(u^n)), \quad \text{éq 4.1-3}$$

where ω is a parameter of relieving, constant on all the field and during all the iterative process,

representing the term $\frac{1}{\tau'(u^n)}$.

Because of the nonconvexity of the function $\tau(u)$, this parameter of relieving necessarily must to check the following condition [bib2], [bib3]:

$$\omega \leq \frac{1}{\max_n \tau'(u^n)} \quad \text{éq 4.1-4}$$

In practice one takes $\omega = \frac{1}{\max_n \tau'(u^n)}$.

By taking of account the approximation [éq 4.1-3], discretization of the second term of the equation [éq 3-2] is expressed in the following way:

$$\int_{\Omega} V \cdot \text{grad } u^{n+1} \psi \, d\Omega = \int_{\Omega} V \cdot \text{grad } u^n \psi \, d\Omega + \int_{\Omega} \omega V \cdot \text{grad } T^{n+1} \psi \, d\Omega - \int_{\Omega} \omega V \cdot \text{grad } \tau(u^n) \psi \, d\Omega, \quad \text{éq 4.1-5}$$

4.2 Treatment of nonthe linearities related on the nonlinear condition of Fourier and thermal conductivity

Nonthe linearity related to the condition of normal flow nonlinear is treated by considering the development with the first order of the function (supposed sufficiently regular) $\alpha(T)$ who is given by:

$$\alpha(T^{n+1}) = \alpha(T^n) + \alpha'(T^n)(T^{n+1} - T^n), \quad \text{éq 4.2-1}$$

where $(.)'$ indicate the derivative of the function $(.)$ compared to its argument.

It appeared necessary to decide on a strategy of discretization of the term $k(T) \text{grad } T$ in the equation [éq 3-2] in order to be able to treat this nonlinearity for the stationary problem which we consider. For that, we adopted the following approximation:

$$k(T^{n+1}) \text{grad } T^{n+1} = k(T^n) \text{grad } T^{n+1} - [k(T^n) - k(T^{n-1})] \text{grad } T^n \quad \text{éq 4.2-2}$$

This discretization is in fact a simplification of the development to the first order of the term $k(T) \text{grad } T$. It is effective being in particular because of the low not linearity of the function $k(T)$ in practice.

Note:

Also let us note that the following purely explicit approximation:

$$k(T^{n+1}) \text{grad } T^{n+1} \approx k(T^n) \text{grad } T^{n+1},$$

also give satisfactory results. This observation was checked starting from several digital experiments.

5 Algorithm established in Code_Aster

The digital diagram employed for the resolution of the problem of reference [éq 2-1], [éq 2-5] is deduced from the variational formulation [éq 3-2] and from the treatment of the various not linearities, [éq 4.1-5], [éq 4.2-1], [éq 4.2-2], discussed in the preceding section.

The algorithm of resolution is consisted the sequence of two successive operations to each iteration of calculation.

Knowing the fields solutions with the iteration $n : T^n$ with the nodes and u^n at the points of Gauss, one seeks the solutions T^{n+1} et u^{n+1} with the iteration $n+1$ as follows:

$$\forall \psi \in V,$$

$$\begin{aligned} & \int_{\Omega} k(T^n) \mathbf{grad} T^{n+1} \cdot \mathbf{grad} \psi \, d\Omega + \int_{\Omega} \omega V \cdot \mathbf{grad} T^{n+1} \psi \, d\Omega \\ & + \int_{\partial_1 \Omega} \gamma T^{n+1} \psi \, d\Gamma - \int_{\partial_3 \Omega} \alpha'(T^n) T^{n+1} \psi \, d\Gamma \\ & = \int_{\Omega} Q \psi \, d\Omega + \int_{\partial_1 \Omega} \gamma T_{ext} \psi \, d\Gamma + \int_{\partial_2 \Omega} q_0 \psi \, d\Omega \quad \text{éq 5-1} \\ & + \int_{\partial_3 \Omega} (\alpha(T^n) - \alpha'(T^n) T^n) \psi \, d\Gamma + \int_{\Omega} [k(T^n) - k(T^{n-1})] \mathbf{grad} T^n \cdot \mathbf{grad} \psi \, d\Omega \\ & + \int_{\Omega} \omega V \cdot \mathbf{grad} t(u^n) \psi \, d\Omega - \int_{\Omega} V \cdot \mathbf{grad} u^n \psi \, d\Omega, \end{aligned}$$

$$u^{n+1} = u^n + \omega (T^{n+1} - \tau(u^n)) \quad \text{éq 5-2}$$

With each iteration, a linear problem of convection-diffusion is solved to obtain the field with the nodes T^{n+1} [éq 5-1], and then a simple on-the-spot correction is carried out to obtain the field at the points of Gauss u^{n+1} [éq 5-2].

The criterion of stop adopted in *Code_Aster* fact of intervening at the same time the two fields solutions: the field of temperature, and the field enthalpy.

The algorithm continues the iterations as long as at least one of the relative variations of reiterated is higher than the corresponding tolerance given by the user:

$$\frac{\left(\sum_{i=1, \dots, nddl} (T_i^{n+1} - T_i^n)^2 \right)^{1/2}}{\left(\sum_{i=1, \dots, nddl} (T_i^{n+1})^2 \right)^{1/2}} > \text{tole 1}$$

$$\frac{\left(\sum_{i=1, \dots, npg} (u_i^{n+1} - T_i^n)^2 \right)^{1/2}}{\left(\sum_{i=1, \dots, npg} (u_i^{n+1})^2 \right)^{1/2}} > \text{tole 2}$$

where *nddl* is the full number of the degrees of freedom to the nodes, and *npg* is the full number of the points of Gauss.

tole1 is well informed under the keyword `crit_temp_rela` keyword factor convergence of the operator `ther_non_line_mo`.

tole2 is well informed under the keyword `crit_enth_rela` keyword factor convergence of the operator `ther_non_line_mo`.

6 Principal options of calculation in Code_Aster

One presents the principal options below of *Code_Aster* specific to the unfolding of the algorithm [éq 5-1], [éq 5-2] above. On the other hand, we will not mention the nonspecific options of *Code_Aster* and which is used in calculation:

- Boundary conditions:

Fourier Linéaire

$$\begin{aligned} & \text{RIGI_THER_COET_R} \\ & \text{RIGI_THER_COET_F} \end{aligned} \int_{\partial_1 \Omega} \gamma T^{n+1} \psi d \Gamma$$

Fourier Non Linéaire

$$\begin{aligned} & \text{RIGI_THER_FLUTNL} \\ & \text{CHAR_THER_FLUTNL} \end{aligned} \int_{\partial_3 \Omega} \alpha'(T^n) T^{n+1} \psi d \Gamma$$

$$\int_{\partial_3 \Omega} (\alpha(T^n) - \alpha'(T^n) T^n) \psi d \Gamma$$

- Elementary matrices and second member:

$$\begin{aligned} & \text{RIGI_THER_TRANS} \\ & \text{RIGI_THER_CONV_T} \\ & \text{CHAR_THER_TNL} \end{aligned} \int_{\Omega} k(T^n) \mathbf{grad} T^{n+1} \cdot \mathbf{grad} \psi d \Omega$$

$$\int_{\Omega} \omega \mathbf{V} \cdot \mathbf{grad} T^{n+1} \psi d \Omega$$

$$\int_{\Omega} [k(T^n) - k(T^{n-1})] \mathbf{grad} T^n \cdot \mathbf{grad} \psi d \Omega$$

$$+ \int_{\Omega} \omega \mathbf{V} \cdot \mathbf{grad} \tau(u^n) \psi d \Omega - \int_{\Omega} \mathbf{V} \cdot \mathbf{grad} u^n \psi d \Omega$$

7 Bibliography

- 1) Duvaut, G., Mechanics of the continuous mediums, Masson, 1990.
- 2) Nochetto, R.H., Numerical methods for free boundary problems, Free Boundary Problems: Theory years Applications, éd. K.H. Hoffmann and J. Spreckels, (Pitman, Boston, 1988).
- 3) Paolini, Mr., Sacchi, G. and Made green, C., Finite Element approximations of singular parabolic problems, Int. J. Numer., Meth. Engng., **26**, pp. 1989-2007, 1988.
- 4) Friedman, A., Variational Principles and Free Boundary Problems, Pure and Applied Mathematics (Wiley-Interscience, New York, 1982).
- 5) Tamma, K.K. and Namburu, R.R., Recent Advances, Trends and New Prospects via enthalpy-based finite element formulations for applications to solidification problems, Int. J. Numer., Meth. Engng., **30**, pp. 803-820, 1990.

8 Description of the versions of the document

Version Aster	Author (S) Organization (S)	Description of the modifications
01/04/00	F. WAECKEL, B. NEDJAR (EDF/IMA/MM N, ENPC)	Initial text