A VARIATIONAL PRINCIPLE FOR FINITE TRANSFORMATION GRADIENT PLASTICITY TO MODEL DUCTILE FRACTURE

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ABSTRACT

This paper presents an approach to predict ductile fracture of real-life structures. It relies on Rousselier's constitutive model to describe plastic void growth, a specific finite strain formulation that preserves energetic properties and a non local theory to deal with strain localisation. It is finally applied to the computation of a notched specimen.

KEYWORDS

ductile fracture, non local formulation, finite strain.

INTRODUCTION

This work proposes a model to predict ductile fracture of real-life steel structures, describing the inception of damaged zones, their propagation and the resulting final structural instability.

The physics of plastic void growth is modelled by Rousselier's model which has already proved its predicting capabilities compared to experimental results [1]. Its yield surface is :

$$\mathrm{F}\left(\boldsymbol{\tau},\, A\,;\, f\right) = \tau_{eq} + \sigma_1\, D\, f\, \exp\left(\frac{\mathrm{tr}\,\boldsymbol{\tau}}{3\sigma_1}\right) - \left(\sigma^y - A\right) \qquad \text{with} \quad \tau_{eq} = \sqrt{\frac{3}{2}\boldsymbol{\tau}^{\mathrm{D}} \cdot \boldsymbol{\tau}^{\mathrm{D}}} \tag{1}$$

$\boldsymbol{\tau}$ denotes Kirchhoff stress, f the porosity, A an isotropic hardening variable and σ^y, σ_1 and D material parameters. There are two main differences with Gurson model, see [2] : the elastic domain is unbounded in compression, as von Mises model, and the yield surface is singular on the hydrostatic axis in traction. Localisation phenomena are expected with such a model. To control them, the resulting high spatial gradients of mechanical fields in the localisation zone have to be explicitly taken into account ; this is achieved by introducing the gradient of the cumulated plastic strain in the model. This non local approach can be expressed as a variational principle for generalised standard materials. To ensure this property in the context of finite strain, a special formulation has to be stated, close to Simo and Miehe's one [3].

Part 1 is dedicated to this specific finite strain formulation while part 2 presents the two main steps of the non local theory. Finally, part 3 aims at demonstrating the operational character of the whole approach.

1. FINITE STRAIN FORMULATION

1.1 Application to Rousselier model

To provide a consistent framework with the variational principle we aim at, classical finite plasticity theory, based on Jaummann rate for instance, can not be used. Actually, we have to build a new theory, see [4], which relies mostly on Simo and Miehe's one [3] and extend the class of generalised standard materials to finite strain. As will be shown, it allows to express the integration of the constitutive relation as a minimisation problem, a crucial point for the application of our variational principle.

It begins with the introduction of a relaxed (stress free) configuration leading to the classical multiplicative split of the total deformation $\mathbf{F} = \mathbf{F}^{\mathbf{e}}\,\mathbf{F}^{\mathbf{p}}$. Then, the free Helmholtz' energy Φ_μ is assumed to be the sum of an elastic energy Φ^{el} that depends only on the elastic strain $\mathbf{e}$ yet to define (isotropic hyperelasticity) and a stored energy Φ^{st} that depends on a hardening internal variable p :

$$\Phi_\mu(\mathbf{e}, p) = \Phi^{\mathrm{el}}(\mathbf{e}) + \Phi^{\mathrm{st}}(p) \qquad \text{with} \quad \mathbf{e} = \frac{1}{2}\left(\mathbf{Id} - \mathbf{F}^{\mathbf{e}}\,\mathbf{F}^{\mathbf{e}^{\mathrm{T}}}\right) = \frac{1}{2}\left(\mathbf{Id} - \mathbf{B}^{\mathbf{e}}\right) \tag{2}$$

$$\begin{cases} \Phi^{\mathrm{el}}(\mathbf{e}) = \dfrac{1}{2}\left[K(\operatorname{tr}\mathbf{e})^2 + 2\mu\,\mathbf{e}^{\mathrm{D}}\cdot\mathbf{e}^{\mathrm{D}}\right] \\ \Phi^{\mathrm{st}}(p) = \displaystyle\int_0^p \mathrm{R}(s)\,ds \end{cases} \tag{3}$$

where K, μ and R denote respectively the bulk and shear moduli and the hardening function. The intrinsic dissipation can be derived for such a choice :

$$Diss = \left(\boldsymbol{\tau} - \mathbf{s}\,\mathbf{B}^{\mathbf{e}}\right)\cdot\mathbf{D} - \frac{1}{2}\mathbf{s}\cdot\left(\mathbf{F}\,\dot{\mathbf{G}}^{\mathbf{p}}\,\mathbf{F}^{\mathrm{T}}\right) + A\,\dot{p} \qquad \mathbf{G}^{\mathbf{p}} = \left(\mathbf{F}^{\mathbf{p}^{\mathrm{T}}}\,\mathbf{F}^{\mathbf{p}}\right)^{-1} \qquad \mathbf{s} \underset{\text{def.}}{=} -\frac{\partial\Phi_\mu}{\partial\mathbf{e}} \qquad A \underset{\text{def.}}{=} -\frac{\partial\Phi_\mu}{\partial p} \tag{4}$$

where $\mathbf{D}$ denotes the Eulerian strain rate. We can notice that a plastic strain measure $\mathbf{G}^{\mathbf{P}}$ and driving forces $\mathbf{s}$ and A associated to $\mathbf{e}$ and p are naturally defined in the process. As the dissipation is required to be zero for elastic evolution, the following stress - strain relation is obtained :

$$\boldsymbol{\tau} = \mathbf{s}\,(\mathbf{Id} - 2\mathbf{e}) \tag{5}$$

Moreover, to ensure a positive dissipation, we assume the principle of maximal plastic dissipation with respect to the yield surface characterised by $\mathrm{F}(\mathbf{s}, A\,; f) = 0$. We can notice that, compared to Eqn. (1), Kirchhoff stress $\boldsymbol{\tau}$ is replaced by the driving force $\mathbf{s}$. Here lies the difference with Simo and Miehe's approach. Nevertheless, thanks to the stress - strain relation Eqn. (5), $\boldsymbol{\tau}$ and $\mathbf{s}$ are close to each other while $\mathbf{e}$ remains small. Such a choice leads to the following evolution equations :

$$\begin{cases} -\dfrac{1}{2}\,\mathbf{F}\,\dot{\mathbf{G}}^{\mathbf{p}}\,\mathbf{F}^{\mathrm{T}} = \lambda\dfrac{\partial \mathrm{F}}{\partial \mathbf{s}} \\ \dot{p} = \lambda\dfrac{\partial \mathrm{F}}{\partial A} \end{cases} \qquad \text{with} \quad \lambda \geq 0 \quad \mathrm{F} \leq 0 \quad \lambda\,\mathrm{F} = 0 \tag{6}$$

Some insights on the advantages of such a formulation compared to a Jaumman rate one are given in [4]. Here, we only mention that these equations are objective (and incrementally objective) since the derivation with respect to time acts on $\mathbf{G}^{\mathbf{P}}$ which is a tensor defined on the initial configuration. Finally, the porosity evolution is based on an eulerian plastic rate :

$$\dot{f} = (1 - f)\,\operatorname{tr}\left(-\frac{1}{2}\,\mathbf{F}\,\dot{\mathbf{G}}^{\mathbf{p}}\,\mathbf{F}^{\mathrm{T}}\right) \qquad \text{with} \quad -\frac{1}{2}\,\mathbf{F}\,\dot{\mathbf{G}}^{\mathbf{p}}\,\mathbf{F}^{\mathrm{T}} = \mathbf{F}^{\mathbf{e}}\,\mathbf{D}^{\mathbf{p}}\,\mathbf{F}^{\mathbf{e}^{\mathrm{T}}} \tag{7}$$

1.2 Integration of the constitutive relation

From now on, we are interested in deriving the time integration of the constitutive behaviour over a single time step. Let us denote respectively by q^-, q and Δq the value of a quantity q at the beginning and the end of the time step, and its increment over the time step. Then, the integration procedure can be stated as : given $\mathbf{e}^-$ (or $\mathbf{G}^{\mathbf{p}^-}$), p^-, f^-, $\mathbf{F}^-$ and $\mathbf{F}$, find $\mathbf{e}$, p, f and $\boldsymbol{\tau}$. For the sake of simplicity, the porosity is treated in an explicit way, while the other variables are dealt with an Euler scheme, classical for plastic constitutive law, see [5]. Let us introduce now the solution for an elastic trial (q^E denotes the value of a quantity q during the elastic trial and $\Delta^E q = q - q^E$) :

$$\begin{cases} p^E = p^- \\ \Delta^E p = \Delta p \end{cases} \qquad \begin{cases} \mathbf{G}^{\mathbf{p}\,E} = \mathbf{G}^{\mathbf{p}-} \\ \Delta^E \mathbf{G}^{\mathbf{p}} = \Delta \mathbf{G}^{\mathbf{p}} \end{cases} \qquad \begin{cases} \mathbf{e}^E = \dfrac{1}{2}\left(\mathbf{Id} - \mathbf{F}\,\mathbf{G}^{\mathbf{p}^-}\,\mathbf{F}^{\mathrm{T}}\right) \\ \Delta^E \mathbf{e} = -\dfrac{1}{2}\mathbf{F}\,\Delta\mathbf{G}^{\mathbf{p}}\,\mathbf{F}^{\mathrm{T}} \end{cases} \qquad \begin{cases} f^E = f^- \\ \Delta^E f = \Delta f \end{cases} \tag{8}$$

Then, the non linear system corresponding to the integration of the constitutive relation reads :

$$\begin{cases} \Delta^E \mathbf{e} = \lambda \dfrac{\partial \mathrm{F}}{\partial \mathbf{s}}\left(\mathbf{s},\, A\,;\, f^-\right) \\ \Delta^E p = \lambda \dfrac{\partial \mathrm{F}}{\partial A}\left(\mathbf{s},\, A\,;\, f^-\right) \end{cases} \qquad \begin{cases} \mathbf{s} = -\dfrac{\partial \Phi_\mu}{\partial \mathbf{e}}\left(\mathbf{e},\, p\right) \\ A = -\dfrac{\partial \Phi_\mu}{\partial p}\left(\mathbf{e},\, p\right) \end{cases} \qquad \begin{cases} \lambda \geq 0 \quad \mathrm{F}\left(\mathbf{s},\, A\,;\, f^-\right) \leq 0 \\ \lambda\, \mathrm{F}\left(\mathbf{s},\, A\,;\, f^-\right) = 0 \end{cases} \tag{9}$$

We do not pay further attention to the resolution of this system, except to mention that special attention should be pay to the singular point of F (corresponding to $\sigma_{eq} = 0$). Finally, the porosity is explicitly computed by :

$$\frac{\dot{f}}{1-f} = \frac{\mathrm{tr}\,\Delta^E \mathbf{e}}{\Delta t} \qquad \Rightarrow \qquad 1 - f = \left(1 - f^-\right)\exp\left(-\,\mathrm{tr}\,\Delta^E \mathbf{e}\right) \tag{10}$$

As above mentioned, one of the advantage of such a finite strain formulation is the expression of the system Eqn. (9) as a minimisation problem. Let us introduce the dissipation potential, where I_K denotes the indicator function of the convex K ($+\infty$ outside K, 0 inside) :

$$\begin{aligned} \Delta_\mu\left(\mathbf{D}^{\mathbf{p}}, \dot{p}\right) &\underset{def}{=} \sup_{\substack{s,A \\ F\left(s,A;f^-\right)\leq 0}} \left(\mathbf{s}\cdot\mathbf{D}^{\mathbf{p}} + A\,\dot{p}\right) \\ &= \sigma^y \dot{p} + \sigma_1\,\mathrm{tr}\,\mathbf{D}^{\mathbf{p}}\left(\ln\frac{\mathrm{tr}\,\mathbf{D}^{\mathbf{p}}}{D\,f\,\dot{p}} - 1\right) + \mathrm{I}_{\mathrm{IR}^+}\left(\mathrm{tr}\,\mathbf{D}^{\mathbf{p}}\right) + \mathrm{I}_{\mathrm{IR}^+}\left(\dot{p} - \frac{2}{3}D^p_{eq}\right) \end{aligned} \tag{11}$$

Then, following [6], it can be shown that Eqn. (9) is equivalent to :

$$\Delta^E \mathbf{e},\, \Delta^E p \text{ are solutions of } \quad \min_{\Delta^E \mathbf{e},\, \Delta^E p}\left[\Phi_\mu\left(\mathbf{e}^E + \Delta^E \mathbf{e},\, p^E + \Delta^E p\right) \;+\; \Delta_\mu\left(\Delta^E \mathbf{e},\, \Delta^E p\right)\right] \tag{12}$$

2. NON LOCAL FORMULATION

2.1 Introduction of gradient terms

In Andrieux et al. [7], a homogenisation scheme was proposed to derive gradient constitutive relations from fully local (microscopic) ones. It allows to take into account potential spatial variations of the macroscopic mechanical fields which may occur with a length scale of the same order as the microscopic scale, that is the scale of an elementary representative volume for the microscopic constitutive relation. Such variations, which can namely occur in presence of singularities or localisation, are not compatible with the assumptions of quasi-periodic homogenisation. Let us apply the main steps of this homogenisation scheme to Rousselier model.

An elementary representative volume is introduced which is made of a collection of N microscopic cells of position $\mathbf{z}_i$, where $\Sigma\,\mathbf{z}_i = 0$. In each of these cells, the material state is described by a microscopic deformation tensor $\mathbf{F}_i$ and the microscopic internal variables $\mathbf{e}_i$ and p_i which obey a microscopic constitutive relation stated in terms of the microscopic potentials Φ_μ and Δ_μ. The simplest localisation relation introducing a spatial variation is assumed :

$$\mathbf{F}_i = \mathbf{F}_\bullet \qquad \mathbf{e}_i = \mathbf{e}_\bullet \qquad p_i = p_\bullet + \mathbf{z}_i \cdot \mathbf{p}_\nabla \tag{13}$$

where $\mathbf{F}_\bullet$, $\mathbf{e}_\bullet$, $p_\bullet$ and $\mathbf{p}_\nabla$ appear as a macroscopic variables. Then, a macroscopic free energy Φ and a macroscopic dissipation potential Δ are derived, depending on the macroscopic variables. Straightforward application of [7] and some simplifications for the dissipation potential (to allow practical computations) leads to :

$$\Phi\left(\mathbf{e}_\bullet, p_\bullet, \mathbf{p}_\nabla\right) = \frac{1}{2}\left[K\left(\operatorname{tr}\mathbf{e}_\bullet\right)^2 + 2\mu\,\mathbf{e}_\bullet^{\mathrm{D}} \cdot \mathbf{e}_\bullet^{\mathrm{D}}\right] + \int_0^{p_\bullet} \mathrm{R}(s)ds \; + \frac{d\,\mathrm{R}}{dp}\left(p_\bullet\right)\mathbf{p}_\nabla \cdot \mathbf{J} \cdot \mathbf{p}_\nabla \tag{14}$$

$$\Delta\left(\mathbf{D}_\bullet^{\mathbf{p}}, \dot{p}_\bullet, \dot{\mathbf{p}}_\nabla\right) = \sigma^y \dot{p}_\bullet + \sigma_1 \operatorname{tr}\mathbf{D}_\bullet^{\mathbf{p}}\left(\ln\frac{\operatorname{tr}\mathbf{D}_\bullet^{\mathbf{p}}}{D\,f^-\,\dot{p}_\bullet} - 1\right) + \mathrm{I}_{\mathrm{IR}^+}\left(\operatorname{tr}\mathbf{D}_\bullet^{\mathbf{p}}\right) + \mathrm{I}_{\mathrm{IR}^+}\left(\dot{p}_\bullet - L_b\left\|\dot{\mathbf{p}}_\nabla\right\| - \frac{2}{3}D_{\bullet eq}^{p}\right) \tag{15}$$

$\mathbf{J}$ is a second-order symmetric tensor which introduces the so-called internal material lengths and depends on the spatial cell distribution. In the case of an isotropic cell distribution, with L_b the distance between the centres of two neighbour cells, it reads :

$$\mathbf{J} = \frac{2L_b{}^2}{13}\mathbf{Id} \tag{16}$$

Note that $\mathbf{z}_i$, $\mathbf{p}_\nabla$ and $\mathbf{J}$ are expressed in the initial configuration : they are lagrangian tensors. Therefore, the internal lengths are implicitly modified by the deformation (induced anisotropy for the non local terms). Finally, it is assumed that at the macroscopic scale, $\mathbf{p}_\nabla$ is equal to the gradient of $p_\bullet$, a choice which is consistent with Eqn.(13) :

$$\begin{cases} p_\bullet = p(x) \\ \mathbf{p}_\nabla = \nabla p(x) \end{cases} \tag{17}$$

2.2 Variational principle

Although the material behaviour is totally defined at the material point scale through the potentials Eqn. (14) and Eqn. (15), the boundary value problem stated over the structure generally does not admit solutions because the state variables $p_\bullet$ and $\mathbf{p}_\nabla$ are linked by relation Eqn. (17) and therefore they are no longer independent. This is however a strong requirement of generalised standard materials. Indeed, this nonlocal relation Eqn. (17) hinders the normality property at the material point scale.

To overcome this difficulty, we propose to put aside the local normality rule, over-constraining, while preserving the formalism of generalised standard materials at the scale of the structure, see [8]. First, the definition of state variables is extended : they become fields over the structure, so that the set of state variables is reduced to the fields $\mathbf{F}$, $\mathbf{e}$ and p. The former variables $p_\bullet$ and $\mathbf{p}_\nabla$ now appear only through different functional operations on the field p, see Eqn. (17). Then, global potentials are defined, which are functions of the state variable fields and their rates :

$$\mathrm{F}\left(\mathbf{e}, p\right) = \int_\Omega \Phi\left(\mathbf{e}(x), p(x), \nabla p(x)\right)\; dx \qquad \mathrm{D}\left(\mathbf{D}^{\mathbf{p}}, p\right) = \int_\Omega \Delta\left(\mathbf{D}^{\mathbf{p}}(x), \dot{p}(x), \nabla\dot{p}(x)\right)\; dx \tag{18}$$

where Ω denotes the body domain in the initial configuration. The generalised standard material formalism is preserved, so that a global constitutive relation can be derived from these potentials Eqn. (18). Thanks to the local character of the elastic strain, the former stress - strain relation is retrieved :

$$\boldsymbol{\tau}(x) = -\frac{\partial \Phi}{\partial e_{\bullet}}\left(\mathbf{Id} - 2\mathbf{e}(x)\right) \tag{19}$$

However, the evolution of the internal variables obeys a non local problem (where appear partial differentiations of functionals with respect to fields and a functional subgradient) :

$$\left(-\frac{\partial \mathrm{F}}{\partial \mathbf{e}}, -\frac{\partial \mathrm{F}}{\partial p}\right) \in \partial \mathrm{D}\left(-\frac{1}{2}\mathbf{F}\,\dot{\mathbf{G}}^{\mathbf{p}}\,\mathbf{F}^{\mathrm{T}}, \dot{p}\right) \tag{20}$$

In spite of the complexity of this evolution equation, the interesting minimisation property Eqn. (12) remains applicable. In the context of an implicit Euler scheme, time integration of Eqn. (20) results in the following minimisation (global) problem, while the evolution of the porosity keeps its former expression Eqn. (10) :

$$\Delta^E\mathbf{e}, \Delta^E p \text{ are solutions of } \min_{\Delta^E\mathbf{e},\, \Delta^E p}\left[\mathrm{F}\left(\mathbf{e}^E + \Delta^E\mathbf{e},\, p^E + \Delta^E p\right) + \mathrm{D}\left(\Delta^E\mathbf{e}, \Delta^E p\right)\right] \tag{21}$$

3. NUMERICAL APPLICATION

To examine the characteristics of such a non local model, a numerical simulation is carried out. A widely studied structure in the context of ductility is an axisymmetrical notched specimen submitted to tension, see figure 1 for the geometry, the loading and the material parameters. A first computation is made with the local model, a second with the non local one.

The integration in the former case is achieved in a classical fashion with a return mapping algorithm based on Eqn. (8) - (10). In the latter case, the integration of the non local constitutive relation relies on the resolution of the minimisation problem Eqn. (21). It presents severe difficulties :

- non differentiability of D (which is positive homogeneous of degree one),
- presence of non linear inequality constraints (indicator function that rules the growth of the cumulated plastic strain),
- large size (as many unknowns as the number of nodes in the mesh).

Therefore, a specific algorithm is required, see [9]. Without entering into further details, let us just mention that it is based on the explicit introduction of the fields $p_{\bullet}$ and $\mathbf{p}_{\nabla}$ at the Gauss points and the dualisation of the resulting constraint Eqn. (17), thus leading to an augmented lagrangian : the relaxed problem is then solved by means of a Newton's method, while BFGS with Wolfe line search is used for the dual one. That's why the expression of the integration as a minimisation problem appears essential. Note that such an algorithm has already proven its efficiency on brittle damage simulation.

The numerical results are presented in terms of the cumulated plastic field around the notch and the horizontal displacement at the notch tip versus the applied force (figure 2). By now, some convergence difficulties are encountered, so that the non local computation does not go as far as the local one. It appears that in this first stage, the results are very close, due to the small characteristic length ($30\,\mu\mathrm{m}$) compared to the characteristic size of the gradients triggered by the notch, as shown by the plastic field picture. To observe a significant difference between both models, we have to wait for localisation to appear, which is achieved with the local model but not yet with the non local one...

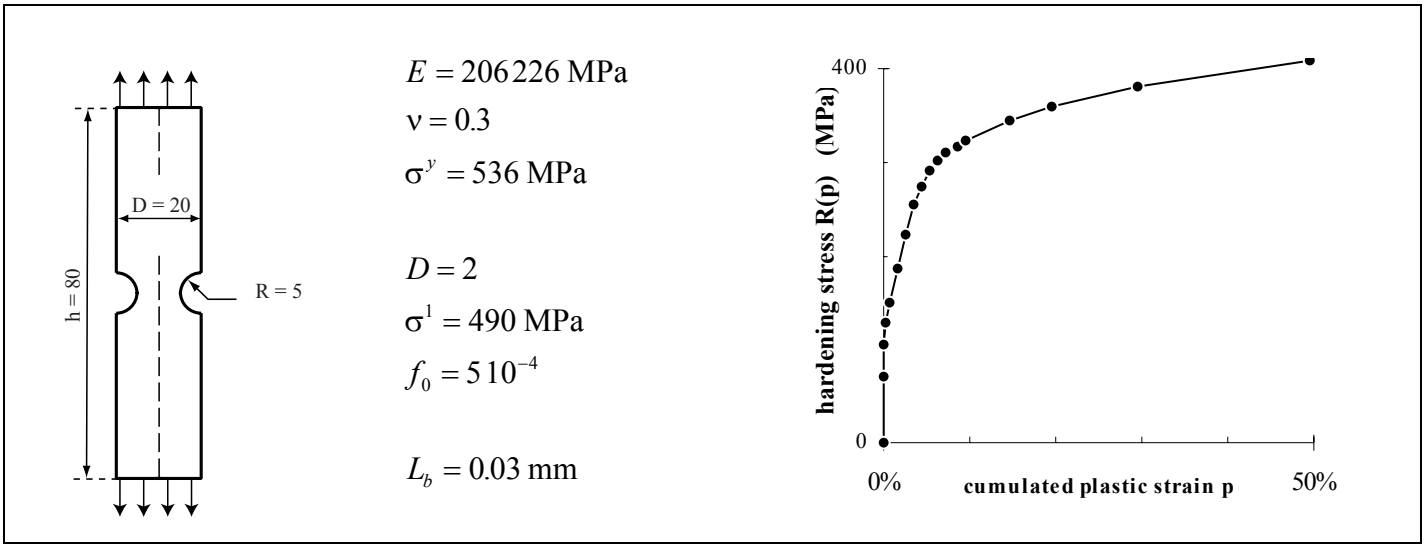

figure 1 - Test problem : geometry, loading and material parameters

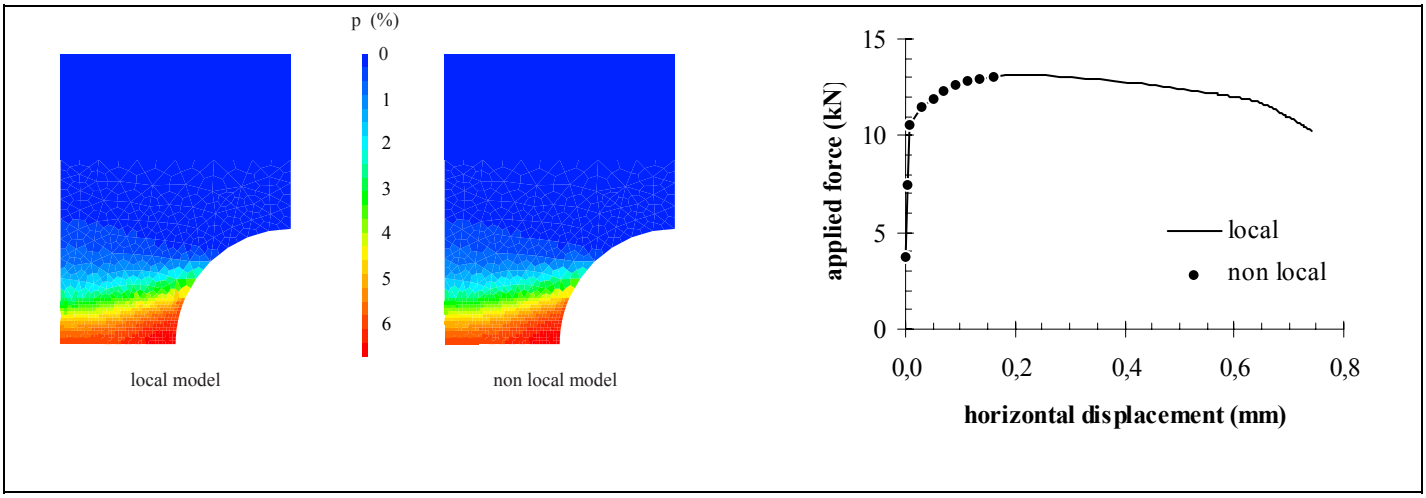

figure 2 - Test problem : local and global responses

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