Nonlocal computational methods applied to composites structures
Norbert Germain, Frédéric Feyel, Jacques Besson

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ABSTRACT
A nonlocal finite element method is used to solve numerical problems appearing when a standard finite element method, coupled with a Newton-Raphson algorithm, is used to model the degradation of organic or ceramic matrix composites structures (OMC or CMC) even under simple solicitations (traction, flexion, ...). The main problem is related to instabilities and localisation, which lead to the divergence of the solver.

In order to overcome these difficulties, a new method is developed. It consists in the use of nonlocal description of the material combined with an arc length algorithm. This ensures a good numerical conditioning which allows the parallelization (using a FETI method) of the calculations and therefore high performance computations.

This set of tools allows to run 3D simulations in order to follow the initiation and the propagation of fracture in cases representative of industrial problems which require very fine meshes.

1 INTRODUCTION
Recent advances in mechanics give a better description of heterogeneous materials like organic or ceramic matrix composites. New sophisticated constitutive equation sets can deal with damage growth. Using these equations, the finite elements method makes it possible to predict the evolution of damage in complex structures, and to prevent their failures. However within this framework, standard finite elements procedures rise a lot of numerical problems. For instance, instabilities and localisations appear, which lead to a quick divergence of the solver.

In this work, a nonlocal model is used to overcome these difficulties. This is not only a new finite element algorithm but set of tools which ensure a good balance between applicability to OMC structures (which exhibit an anisotropic (viscous-) elastic damageable behavior), high performance computation, and of course, a good numerical conditioning.

The main parts of the method are:
- A nonlocal model including damage implicit gradient (instead of a local method), to solve the problem of mesh dependency while remaining applicable in anisotropic/heterogeneous problems,
• An optimized arc length algorithm, to solve the resulting nonlinear equations and to deal with unloadings,
• A FETI's like method allowing nonlocal parallel computations.

2 EXAMPLES OF NUMERICAL PROBLEMS
In this section, a numerical example is presented to emphasize the need of such methods. The simulation consists of a three points bending test (fig. 1) carried out on a specimen made of CMC, which is modelled (taking into account the symmetry) using four different meshes having different element sizes.

At the macroscopic level (fig. 2), all computations end when the maximum load is reached. This is likely to be a related to a snap-back phenomenon. At microscopic level (fig. 3), the isocontour plots show that whatever the mesh, the deformation is localized within a region whose width correspond to the element size.

This simple example clearly shows the two main problems encountered when using damage models: (i) structural instabilities, (ii) meshes sensitivity. Clearly, both problems must be solved to obtain reliable results. In the following, the different ingredients needed to reach this goal, are presented.

figure 1: Test specimen and boundary condition

figure 2: Force- Displacement curve
Different ways have been explored to solve the localization problem. A nonlocal method based on an implicit gradient formulation was chosen (Peerlings, [1]), where the nonlocal variable is the damage $D$.

Let us consider the following local problem:

\[
\begin{align*}
\text{div}(\sigma) &= 0 \quad \text{in } \Omega \\
\sigma &= (1 - D)C : \varepsilon \\
D &= g(Y) \\
Y &= \frac{1}{2} (\varepsilon : C : \varepsilon) \\
\varepsilon &= \frac{1}{2} \nabla_s (u) \\
u &= u_i \quad \text{on } \Gamma_u \\
\sigma : n &= F \quad \text{on } \Gamma_f
\end{align*}
\]

The nonlocal equivalent problem is defined by:

\[
\begin{align*}
\text{div}(\tilde{\sigma}) &= 0 \quad \text{in } \Omega \\
\tilde{\sigma} &= (1 - \tilde{D})C : \varepsilon \\
\tilde{D} &= g(Y) \\
\tilde{Y} &= \frac{1}{2} (\varepsilon : C : \varepsilon) \\
\tilde{\varepsilon} &= \frac{1}{2} \nabla_s (u) \\
u &= u_i \quad \text{on } \Gamma_u \\
\tilde{\sigma} : n &= F \quad \text{on } \Gamma_f
\end{align*}
\]
An additional boundary value problem describes the evolution of the nonlocal damage variable $\tilde{D}$:

$$\begin{align*}
\tilde{D} - c\nabla^2 \tilde{D} &= D \quad \text{in } \Omega \\
\frac{\partial \tilde{D}}{\partial x_i} &= 0 \quad \text{on } \Gamma
\end{align*}$$

This new formulation has been implemented and tested in a finite elements code.

This model lacks some important features of composite materials, especially the induced damage anisotropy. A new model formulation is needed to account for this effect.

4. ARC LENGTH ALGORITHM

To solve instabilities and divergence problems, an algorithm based on an arc length method is used (Zienkiewicz, [2]). A load parameter $\lambda$ is introduced as a new unknown of the problem. It is assumed that the total load is proportional to $\lambda$ and a load direction $F$. The problem to be solved is:

$$\begin{align*}
g(p,\lambda) = q_i(p,\lambda) - q_{ext}(\lambda) &= 0 \\
h(p') &= L^2
\end{align*}$$

Where $q_i$ is the internal reactions vector and $q_{ext}$ the external reactions vector (equal to $\lambda F$). $h$ is a control function, $p'$ is a sub-set of $p$ (watch points). $p$ are the problem unknowns: displacements and nonlocal damage. The solution scheme is based on an iterative Newton-Raphson algorithm; therefore, the problem is to find the unknown increments $\delta p$ and $\delta \lambda$ at a given increment:

$$\begin{align*}
p &= p_0 + \delta p \\
\lambda &= \lambda_0 + \delta \lambda
\end{align*}$$

where $p_0$ and $\lambda_0$ are the values at the beginning of the increment. Such as:

$$\delta p = -K_0^{-1} g(p_0,\lambda_0) - \partial \lambda K_0^{-1} q_0^1$$

Where:

$$\begin{align*}
K_0 &= \frac{\partial q_i}{\partial p}(p_0,\lambda_0) \\
q_0^1 &= \frac{\partial q_i}{\partial \lambda}(p_0,\lambda_0) - \frac{\partial q_{ext}}{\partial \lambda}(\lambda_0)
\end{align*}$$

In the literature, a lot of methods have been developed (Alfano, [3] - de Borst, [4] - Hellweg, [5]) but none of them is always satisfying. It has been decided to develop an oriented object implementation of this class of algorithms, in order to test existing method and implement new ones easily.

First, two algorithms have been tested where $h$ is equal to:

$$h(p') = \Delta p'^T \Delta p' \quad \text{(Alfano, [3])}$$
The chosen control function can lead to an order two polynomial system (eq. 8): another criterion is needed to choose between the two roots.

The chosen control function can lead to an order two polynomial system (eq. 8): another criterion is needed to choose between the two roots. For that purpose, different methods can be used:

- Choose the one which minimizes the angle between the previous approximation and the new one (Alfano, [3]),
- Choose the one which minimizes the residual (Hellweg, [5]).

It appears through different tests that the "better" solution seems to be the second order equation coupled with an angle minimization technique. The watch points $p'$ correspond to nodal displacements where damage grows rapidly (i.e. nodes where increments of $\tilde{D}$ are large). This method is thought to give a good balance between step size and numerical conditioning.

5. PARALLEL COMPUTATION

The increase of the structures and behaviours complexity increase the simulation time. The parallelization of the finite elements code becomes necessary. This is especially true for nonlocal models as they need more unknowns. Moreover, performing simulations with damage models requires a large number of time steps. Therefore, parallelizing the nonlocal finite elements method is a possible solution to reduce the computation time.

First, the arc-length algorithm needs to be parallelized. Inside each sub-domain $O_i$ of $O$ ($\Omega = \bigcup_{i=1}^{s} \Omega_i$), the value of the load parameters $\gamma_i$ is computed and $\gamma$ is equal to the minimum value. Possibly, it will be necessary to develop another method in order to select a less pessimistic load increment.

Next, the nonlocal method has been parallelized. The method is based on a FETI's algorithm (Farhat & Roux, [6]), which consists, for local problems, in giving new unknowns: the forces $a_i$ to be enforced on domain boundaries to ensure displacement continuity across sub-domains. The forces $a_i$ are estimated with an iterative method.

In the case of nonlocal problem, equilibrium and continuity have to be ensured for both displacement and damage nodal variables. The difficulty is that these entities do not have the same dimension. Thus, the parallelization of the nonlocal equations needs the use of a FETI's extension to multifields problem.
CONCLUSION

The first results given by the nonlocal model and the arc-length algorithm seem to be promising. The problems of localisation and instabilities have been overcome. The parallelization and the generalization of these methods to organic or ceramic matrix composite will allow simulation of industrial structures in order to predict the evolution of damage and to prevent their failures.

REFERENCES