Composite materials calculation using HPC-based multiscale technique.

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***Abstract*—Calculating the behavior of large composite material structures still demanding large computational effort. The solution proposed to tackle the problem is to combine multi-scale homogenization methods with the high performance computational techniques available. This PhD work aims to implement inside the Alya HPC-code a multi-scale algorithm capable of solving this kind of problems in an efficient and accurate way.**

I. Introduction

Simulation of large structures made of composite materials continues to be a challenge even with the huge development of computational technology (see [1]). This PhD work is focused on implementing a technique based on multi-scale calculation taking advantage on the high performance techniques in order to obtain accurate solutions of large non-linear problems.

In the present work we give a short explanation of the multi-scale method and we discuss the basics on material non-linearities and the work flow that is been taken.

II. Multi-scale calculations

Generally the problems in mechanical analysis are expressed in a virtual work form and then are solved by the finite element method. In this case, for simplicity, taking a steady state problem and assuming the small deformation approach, the equations without considering boundary conditions can be state (see [2]) as:

$$\int_V \overline{\boldsymbol{\tau}} \cdot \delta\overline{\boldsymbol{\epsilon}}\, dV = \boldsymbol{\mathcal{R}} \tag{1}$$

where $\overline{\boldsymbol{\tau}}$ is the Cauchy stress tensor, $\delta\overline{\boldsymbol{\epsilon}}$ is the virtual strain and $\boldsymbol{\mathcal{R}}$ is the external virtual work done.

The problem above consist on solving for the stress field $\overline{\boldsymbol{\tau}}$ that satisfies the virtual work Eq. (1) for every virtual strain $\delta\overline{\boldsymbol{\epsilon}}$. Commonly stress $\overline{\boldsymbol{\tau}}$ and strains $\overline{\boldsymbol{\epsilon}}$ are expressed as functions of the displacement $\overline{\boldsymbol{u}}$, i.e.:

$$\overline{\boldsymbol{\tau}} = \overline{\boldsymbol{\tau}}(\overline{\boldsymbol{u}}), \quad \overline{\boldsymbol{\epsilon}} = \overline{\boldsymbol{\epsilon}}(\overline{\boldsymbol{u}}), \tag{2}$$

and a constitutive law equation like

$$\overline{\boldsymbol{\tau}} = \mathbb{C} : \overline{\boldsymbol{\epsilon}}, \tag{3}$$

is added. Here $\mathbb{C}$ is the four-order constitutive tensor and depends on the material. By this way the problem is to find the displacements $\overline{\boldsymbol{u}}$ that satisfy (1) and (3) at the same time.

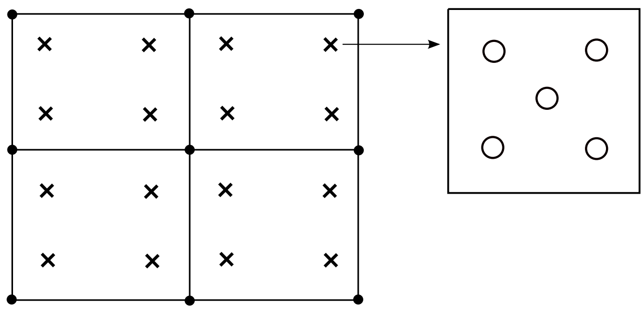

Fig. 1. Multi-scale calculation representation. A general structure is discretized in a coarse mesh and during the assembly process at each integration point a problem over a representative volume element (RVE) that contains the micro-structure information of the composite is solved.

At this point it is possible to notice that during the assembly process for obtaining a detailed calculation of the solid that is being treated, the constitutive $\mathbb{C}$ tensor should be defined on every point of the finite element mesh. Moreover, $\mathbb{C}$ depends on $\overline{\boldsymbol{\epsilon}}$ and on the history making that the problem becomes non-linear and more difficult to solve.

Having this in mind, calculating the behavior of composite materials applying the finite element technique directly, specially on large domains such as an aircraft panel, can derive in an extremely large system of equations due to the huge number of elements used to represent such heterogeneous domain. On the other hand memory, requirements become large when non linearities such as damage and plasticity should be modeled and a huge number of variables should be stored for every element in the mesh.

This situation brought scientist and engineers to developed the multi-scale calculation method capable to afford this problem reducing the computational cost and, at the same time, remaining the accuracy.

Multi-scale calculation method consist of reducing an heterogeneous problem to an homogeneous one, such process is outlined at Fig. (1). During the assembling stage of the global matrix that corresponds to the macro-scale problem, in each integration point a PDE over a representative volume element (RVE) is solved giving average values of $\mathbb{C}$ and $\overline{\boldsymbol{\tau}}$.

It is important to remark that the RVE problem considers the periodical micro-structure of the composite material and the boundary conditions that are given by the macro-problem.

A considerable part of this work is to acquire the capacity of modeling the most important phenomenons that occurs in composite materials which are going to be solved over each RVE during the multi-scale calculations. In the present work a damage model it is explained.

III. Damage model

Continuum damage models are widely used to represent the complex behavior of materials when they are subjected to large loads and they are out of the elastic and linear range.

During a multi-scale simulation on every RVE that it is subjected to large loads a damage model is going to be activated. By this way, an isotropic damage model based on [3] has been implemented in order to understand the basics of this phenomenon.

The general isotropic damage model (see [4]) can be formulated as:

$$\overline{\boldsymbol{\tau}} = (1-d)\mathbb{C}_0 : \bar{\boldsymbol{\epsilon}}, \tag{4}$$

where d is the damage variable ($d \in [0,1]$) and $\mathbb{C}_0$ is the undamaged constitutive tensor. Also a damage criterion, which determines when the material starts damaging, should be defined. For this case it adopts an inequality form like:

$$F(\tau, r) = G(\tau) - G(r) \leq 0, \tag{5}$$

where G is a function that depends on the material properties, τ is a scalar variable that determines the way of how the stress tensor $\overline{\boldsymbol{\tau}}$ produce damage. When that inequality stops holding then the material starts damaging increasing the values of d.

In this work a 1D model was implemented using the finite element approach in order to test the objective response of the model, this means that the solution should not depend on the element size of the mesh. In Fig. 2 two solutions for a 1D case subjected to displacements boundary conditions are shown for two meshes that differ on the node number. As it can be seen, objectivity for this case has been achieved.

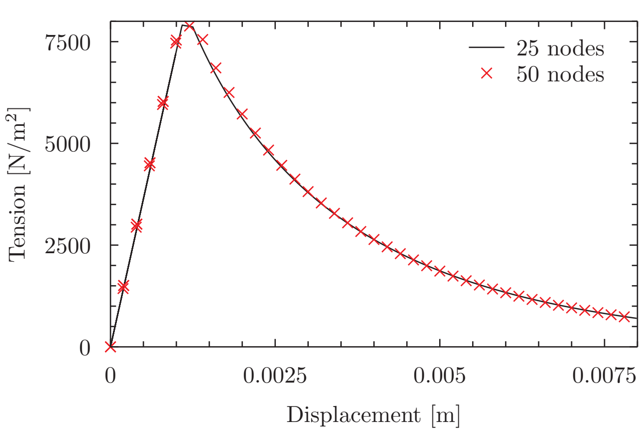

Fig. 2. Objectivity in a 1D finite element model implemented for damage calculations.

In Fig. 3 a 2D damage result is shown. At this point, some difficulties have been observed on the convergence of the Newton-Raphson method used for solving the non-linear equations. This is produced because the residue of the non-linear equations reaches a zero derivative point which is a situation where Newton-Raphson schemes fail. To solve this an Arc-Length method (see [5]) is been implemented and tested in order afford more complex problems.

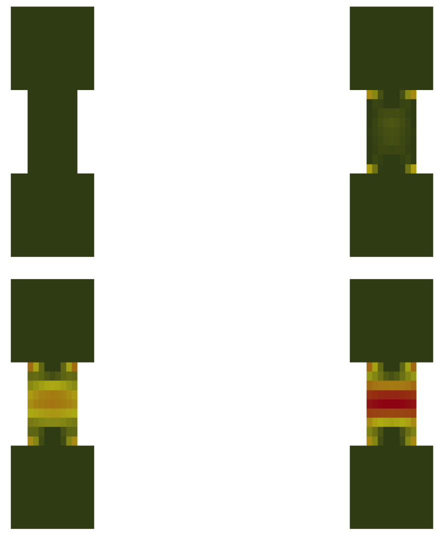

Fig. 3. Damage calculation in a 2D traction test device.

IV. Conclusions

Multi-scale calculation concept has been presented here as the main line of work. The technique will be applied inside the Alya HPC-code after composite materials calculations have been done in smaller scale codes and tested. In this stage non-linear behavior that results from damage, plasticity and large-deformations should be dominated in order to be applied on multi-scale.

Up to now small scale codes have been developed in order to calculate the non-linear behavior of materials and to measure the performance of the numerical methods involved. The most important code takes advantage of the PETSc library to perform a domain decomposition finite element algorithm and to solve large systems of equations and problems that require big amounts of memory.

References

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