An introduction to FE2 multi-scale methods and why HPC is so crucial.

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I. METHODOLOGY

There is no doubt that composite materials are widely used nowadays in almost every engineering areas, mainly because of their excellent properties such as their high resistance, low weight and cost. For this reason it is useful to study their behavior in order to increase their reliability and produce better designs.

There are two main ways of studying composite materials structures. The first and the oldest one is to build a real prototype with the material and to perform experiments, for example, to measure the prototype resistance with a traction test. The second way is to create a computational model applying physical laws and then to predict how it would behave.
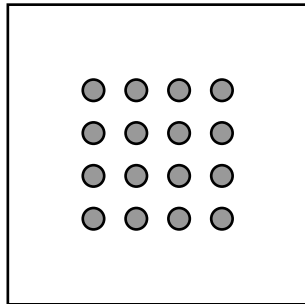

Fig. 1: Representation in two dimensions of a classical composite material structure. In this case the structure is made of two different materials (fibers inside a matrix).

The experimental method can be very accurate because we use directly the real material but it has the counterpart of being expensive because for almost every experiment a new prototype should be manufactured. This is a very slow process specially for those cases where an optimal and reliable design is being searched.

The problem of the cost and speed of the experimental method can be solved with the computational simulations. They involve to develop physical models in order to get accurate solutions, this can be a difficult task depending on the composite material we are dealing with. The most common numerical procedure used in this field is the *finite element method* (FEM) that is combined with constitutive laws to relate the physical variables of the problem. These laws relate the stresses σ and the strains ϵ that are defined at every point in the domain ant they are obtained through experiments.

Composite materials are characterized for being composed of two or more homogeneous materials. In Fig. 1 we represent an example in two dimensions of a typical arrangement of two different materials: a micro structure made of fibers inside a matrix. The distribution and the properties of each material determine the property of the final arrangement. This is a clear example of why computational simulations can allow to find faster an optimal design of a structure because the wide spectra of design options that exist.

In view of what is represented on Fig. 1 it is clear that using the FEM method directly to solve the complete problem can end in a large computational problem that is not feasible to be solved. This is due to the strong difference between the scales that are inside the problem: the structural macroscopic scale and the microscopic scale. A simple explanation of why this happens can be understand by imagining that if at least one finite element is set inside each fiber, then, a large number of finite elements would be needed to discretize the whole problem. Even for a supercomputer the size of this problem can be out of the calculation scale for several orders of magnitude.
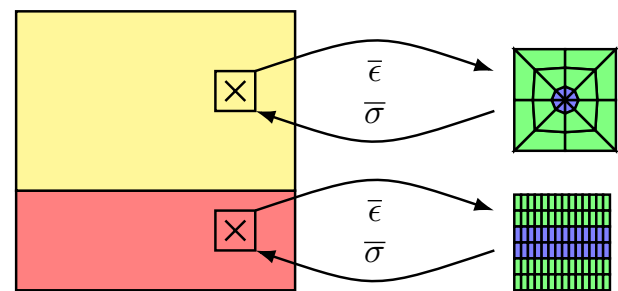

Fig. 2: Representation of the FE2 multi-scale method process. In this example the structure is composed of two different composite materials microstructures (two layers of matrix and fibers with different orientation angles.

To deal with this, the *multi-scale* techniques can be used. The basic idea is to decompose the original problem into two smaller ones: a *macroscopic* and a *microscopic* problem. The macroscopic problem is solved with a coarse FEM mesh and the materials that conforms these elements are homogeneous with constitutive laws obtained using the microscopic model.

For this work we are going to apply the FE2 multi-scale method, here the FEM is applied at both scales which means that in the microscopic scale also the FEM is used to get these properties needed by the macroscopic model. In Fig. 2 we outline this process for a macroscopic structure that is build with two different microscopic structures.

Finally, we should give a briefly idea of the physical models that we are dealing with. For the macroscopic scale we consider the set of equations:

$$\begin{cases} \text{div } \overline{\sigma} = 0 \\ \overline{\sigma} = \langle \sigma \rangle \\ \overline{u} = \overline{u_d} \text{ in } \Gamma_d \\ \overline{\sigma} = \overline{\sigma_n} \text{ in } \Gamma_n \end{cases}$$

where the first is an *equilibrium equation* and the second one is a constitutive law that is obtained using the microscopic model. This is the main difference between the classical single-scale and the multi-scale approach. The others equations are boundary condition equations like in all classical problems.

The macroscopic quantities are calculated with the micro-scopic model that is defined as:

$$\begin{cases} \text{div}\sigma = 0 \\ \sigma = f(\epsilon) \\ \langle \epsilon \rangle = \overline{\epsilon} \end{cases}$$

here, the first is an equilibrium equation and the second are the constitutive laws of each of the materials that conform the microscopic structure, for this problem these laws are known. The third equation is a supposition and means that the average of the strain field ϵ is equal to the macroscopic strain $\overline{\epsilon}$. This crucial assumption determines which boundary conditions can be imposed in the microscopic model.

The boundary conditions that can be set in the microscopic model are:

- Periodic

- Uniform strain

- Uniform stress

Each boundary condition produce a different result at the microscopic level, and consequently, at the macroscopic one. Their accuracy of the boundary conditions depends on the problem that is being solved. For example, in the case of aeronautics composite materials, the *periodic* boundary conditions generally give the most accurate results because the microstructure is near to be periodic and the microscopic model is subjected to a similar constrain.

In Fig. 3 we outline the results of a microscopic structure subjected to different boundary conditions.

II. STRATEGY PROPOSED

The strategy for solving this problem is a distributed memory approach due to the large amount of memory that should be used specially in non-linear problems. In Fig.4 we show the computational scheme that we are going to apply in order to deal with the memory problem. This last consists in applying a domain partition on the macroscopic

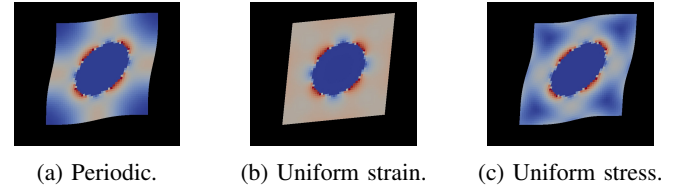(a) Periodic.   (b) Uniform strain.   (c) Uniform stress.

Fig. 3: Results of a microscopic problem subjected to different boundary conditions.

problem and solve each problem in a different node of a cluster. In this case all of the sub domains are communicated with the others using the MPI protocol, each of them works jointly with a microscopic code that performs the constitutive calculations using the FEM. We plan to add another level of parallelization at the microscopic problem using a *shared memory* memory approach, for example, using *OpenMP* to parallelize the matrix-vector products for solving the linear systems or for performing the assembly of the matrices and RHS.
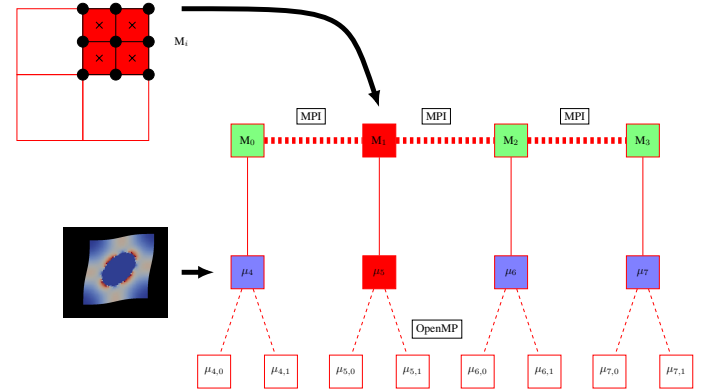

Fig. 4: Distributed strategy that we propose to solve the FE2 problem. In this case the macroscopic problem is divided in four domains and each one is solved in a distributed way among four nodes of a cluster. In each of these nodes an independent microscopic problem is also being solved for retrieving the macroscopic average quantities. The microscopic problem can be parallelized also in a share memory approach considering that each node has more than one CPU.

III. AUTHOR BIOGRAPHY

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