Universitat Politècnica de Catalunya
Master on Numerical Methods in Engineering

Industrial Training

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Project: ***A coupling procedure for the diffusion and mechanical problem***

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Introduction

In engineering many times it is necessary to simulate processes in which more than one phenomenon occurs simultaneously and the behavior of one of them affects the other one. This is the case for many electro-sensitive materials and biological tissues, where the diffusion of an electric charge or a chemical substance affects the mechanical solid response to its boundary conditions.

The purpose of this project was to develop a code to perform a fully coupled simulation of a non-linear elastic material with a diffusive chemical variable, which can be of interest for example in chemical diffusion in battery banks or biomechanic simulations.

In order to do so, firstly, a vast bibliographical research was performed to better understand the behavior of non-linear materials and methodologies to couple diffusion problems with mechanic ones. Once the concepts were clear, the solver which will be explained in the following section, was coded in Matlab.

Methodology

The problem involved solving two coupled partial differential equations, one responsible for the mechanical behavior of the solid and another one for the diffusion of a certain concentration of substance, both of them occurring on the same physical domain. In order to tackle the problem, firstly each of the involved PDE's were solved separately. In the following subsections, the governing equations and the methodology used to solve them are briefly explained.

Mechanical problem

The mechanical behavior of a solid can be represented with the following quasi-static momentum balance equation:

$$\mathbf{0} = \nabla \cdot \boldsymbol{P} + \boldsymbol{F}^{\varphi}$$

where $\boldsymbol{P}$ is the first Piola-Kirchoff stress tensor and $\boldsymbol{F}^{\varphi}$ are the body forces. Note that as the model do not account for a transient behavior, the divergence of the stress should be in equilibrium with the body forces.

After weighting, integrating by part and discretizing the spatial domain, the following residual form was obtained:

$$R_J^{\varphi} = \mathop{\mathsf{A}}_{e=1}^{n_{el}} \int_{\Omega^e} \nabla N_j^{\varphi} \cdot \boldsymbol{P} d\Omega - \int_{\Omega^e} N_j^{\varphi} \boldsymbol{F}^{\varphi} d\Omega - \int_{\Gamma_P^e} N_j^{\varphi} \bar{\boldsymbol{T}}^P d\Gamma = 0 \tag{1}$$

where N^{φ} are the shape-functions for the approximation of the mechanical displacements $\boldsymbol{\varphi}$ and $\bar{\boldsymbol{T}}^P$ are the Neumann boundary conditions. The symbol A represent the assembly of the local residual vectors into the global one.

In order to solve the problem, the material model had to be defined. In this project, working with non-linear elastic models was of special interest, finally settling for a Neo-Hookean model as it is capable of reproducing rubber and biological tissue like materials. Its fundamental constitutive law is given by the strain energy equation

$$\Psi = \frac{1}{2}\lambda(ln\ J)^2 - \mu(ln\ J) + \frac{1}{2}\mu(tr\boldsymbol{C} - 3)$$

where λ and μ are material constants (first Lamme parameter and bulk modulus), J is the Jacobian and $\boldsymbol{C}$ is the Cauchy-Green deformation tensor.

But to solve the problem and expression for the first Piola-Kirchoff stress was needed, which was obtained by deriving the energy function with respect to the deformation gradient.

$$\boldsymbol{P} = \mu \boldsymbol{F} + (\lambda\, ln(J) - \mu)\boldsymbol{F}^{-1}$$

Note, that the material is capable of volumetric growth, and therefore a multiplicative decomposition of the deformation gradient is done in order to take into account this change in the mechanic behavior.

$$\boldsymbol{F} = \boldsymbol{Fe} \cdot \theta\, \boldsymbol{I}$$

In order to solve the problem, the equations were solved iteratively through the Newton-Rhapson method.

Diffusion problem

The diffusion of a certain concentration is governed by the following transient balance equation:

$$\dot{\phi} = \nabla \cdot \boldsymbol{Q} + F^{\phi}$$

where $\dot{\phi}$ is the temporal variation of the concentration, $\boldsymbol{Q}$ is the corresponding flux and F^{ϕ} is the source term.

When weighted, integrated and discretized, the residual form was obtained

$$R_I^{\phi} = \mathop{\mathbf{A}}_{e=1}^{n_{el}} \int_{\Omega^e} N_i^{\phi} \frac{1}{\Delta t}[\phi - \phi_n] d\Omega + \int_{\Omega^e} \nabla N_i^{\phi} \cdot \boldsymbol{Q} d\Omega - \int_{\Omega^e} N_i^{\phi} F^{\phi} d\Omega - \int_{\Gamma_Q^e} N_i^{\phi} \bar{T}^Q d\Gamma = 0 \quad (2)$$

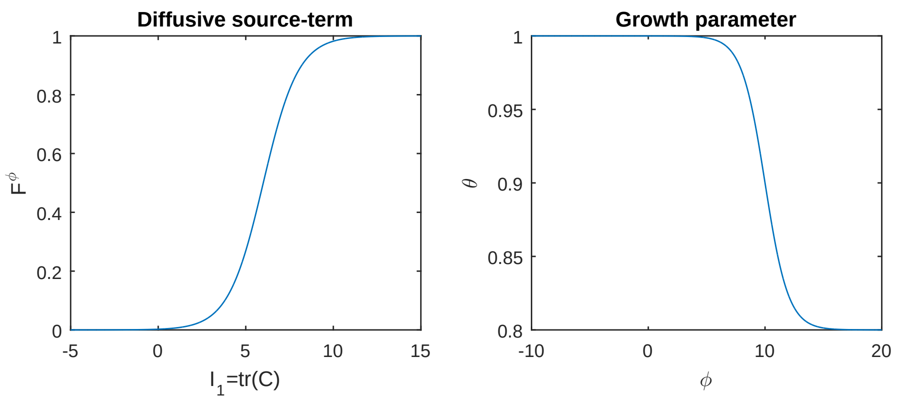
where ϕ and ϕ_n correspond to the concentration in the current and previous time-step and $\bar{T}^Q$ are the Neumann boundary conditions. Note that for the temporal discretization, a fully implicit integration was used for numerical stability reasons.

Coupled problem

In order to couple this problems in both directions, two law were defined. In one hand, the concentration of the substance introduces a volumetric shrinking in the solid mechanic behaviour. In the other, an increase in the deformation promotes the generations of substance through the diffusive source term. To control and limit the effects of the coupling, two sinusoidal functions were defined:

$$\theta = 1 - \frac{x}{1 + e^{-y(\phi - z)}} \qquad F^{\phi} = \frac{a}{1 + e^{-b(I_1 - c)}}$$

where x, y, z, a, b, c are constants used tune the center, slope and amplitude of the functions.



To solve the problem, the residual equations were linearized with respect to both variables, obtaining a coupled $\boldsymbol{K}$ matrix, which was used with a Newton-Rhapson method to solve iteratively.

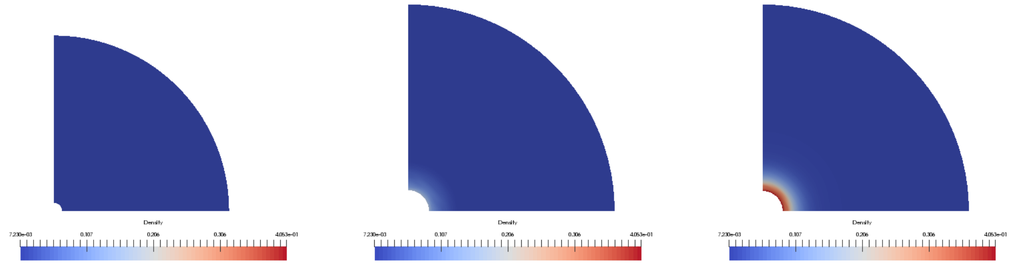
Pre and Post processing

In order to work with the finite element solver developed in Matlab, a GiD problem type was coded to export the finite element mesh and the boundary conditions in a suitable format for this solver in particular.

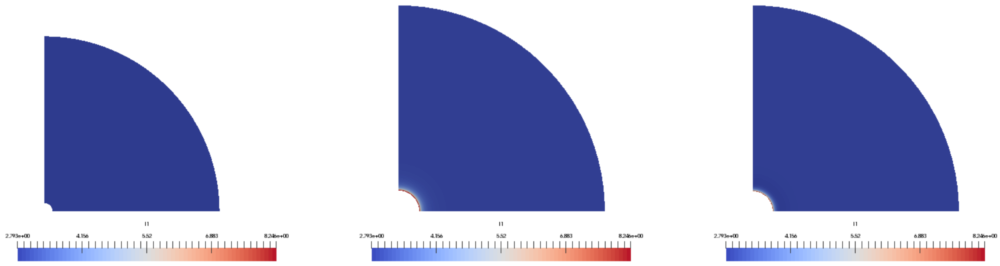
For the visualization of the results, another code was created in order to export the node variables along with other interpolated information to a Paraview format.

Results

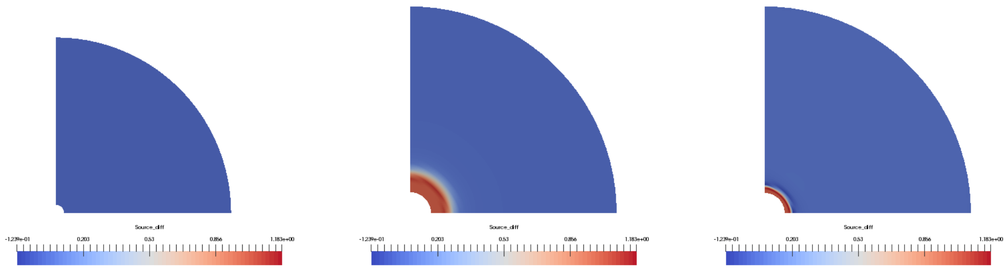
In this section, some time-steps from a fully coupled simulation can be observed.



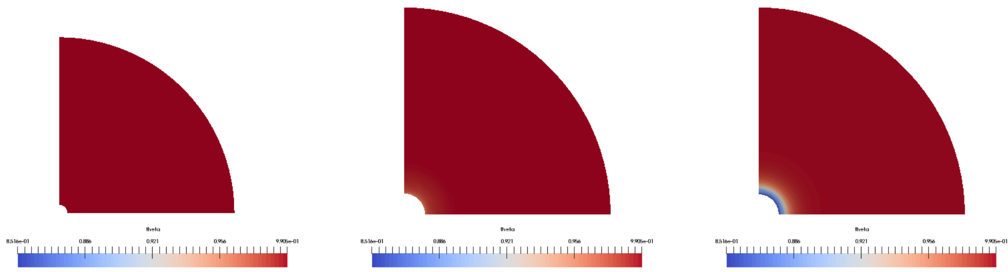
Concentration evolution (time-steps=0,10,20)



I_1 *evolution (time-steps=0,10,20)*



Diffusive source term evolution (time-steps=0,10,20)



Growth parameter evolution (time-steps=0,10,20)

For this example, Dirichlet boundary conditions were imposed to the displacement in the initial steps of the time integration, displacing radially the external boundary and limiting the horizontal and vertical displacements of the left and bottom sides of the domain. The diffusive part of the problem did not have any constrain but the initial conditions.

It can be observed how when the initial displacement is imposed, the mesh deforms following the non-linear expected behavior, but no source term or θ evolution is seen. When a trigger point is reached, the diffusive evolution produces a decrease in the growth parameter and the deformation induces the source term increase. The growth evolution results in a deformation response that reduces the first invariant and consequently the diffusive source term.

Conclusions about the training experience

Once the project topic was defined, bibliographic research was done in order to understand the basics of the field of interest. Understanding the problem and the state of the art proved to be not only challenging but stimulating and useful, as few hours were dedicated to non-linear elasticity during the course.

The writing of reports was done in parallel to the code development and proved to be practical as it helped to better organize the tasks to be done and correct mistakes on the go.

Many hours were devoted to debugging of the codes when no convergence was reached or incoherent results were obtained. This part proved to be the most frustrating and slowing one, although when positive advances it was really rewarding. It is important to remark that in this situations, the expertise of the supervisor became fundamental, giving advice and ideas to identify the root of the problems and how to solve them.

The fact of doing this work while simultaneously taking courses for the 3rd semester was challenging for two reasons: the superposition of delivery dates of different projects (course and industrial training) and the managing of the daily schedule (which had to be adapted for both activities). It was not until the master courses were completed that the greatest and fastest advances were achieved.

Finally, this months of work were of great value from a personal perspective. Although having several years of working experience in the engineering field, I have never done pure academic research before. This project was useful to experience the pros and cons of this type of activity and it also helped to increase the understanding on diverse fields in computational mechanics I had.