EM MSc Computational Mechanics: Industrial training report

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1 Introduction

Inverse analysis is a powerful tool that can be used to extract data that the direct FEM analysis assumes known, such as material characteristics or forces acting over the domain. The development of new devices and algorithms to track displacements and deformations in biological tissue (up to the cellular level) has brought the need to apply these data retrieval methods to the biomechanics field. In the case relative to the work done during this industrial training, the need to compute displacements and forces involved in the embryogenesis of the *Drosophila melanogaster* from a set of displacements obtained through images. From this starting point, a complete FEM code has been developed to take the evolution of a numerical mesh (already provided) and compute unknown displacements and forces in an easy-to-read format. The code allows the user to modify the parameters of the model at their will (visco-elastic model, material stiffness, dimensions of study, forces considered, etc), and is easily understandable thanks to a User Guide that details anything that a future user of the code needs to know in order to perform the tests.

2 Objective

The main objective was the development of an Inverse FEM analysis tool that could compute the forces acting on a given mesh through a set of known displacements, under a set of variable parameters, and in a short time. The model had to allow the user to choose several parameters:

- Viscoelastic model: Kelvin-Voigt or Maxwell
- Dimension: 2D plane strain or 3D extrusion of the geometry
- Set of forces: contractile dipoles, bulk pressures, contractile "pressure-like" forces
- Having the previous forces known *a priori* or unknown

- The regularization parameters λ that are used so as to avoid having spoiled results due to the multiple number of possible solutions
- Material parameters: Young modulus, poisson ratio, viscosity
- Time integration parameters: total integration time, number of time steps, step-size, θ
- Collapse of elements so that several elements share the same value of forces

And it should also allow the use of different meshes by means of providing the necessary mesh data (connectivity and node positions at every time-step).

The results had to be saved in *vtk* format, allowing the data to be saved in an efficient way and to be visualized with *Paraview* (free post-processing software, widely used in the scientific community).

The tool had to be easy to understand, so somebody without notions of the finite element method could use it to perform numerical tests.

3 Results

The final product is made of:

- A 18 pages long User Guide, detailing the mathematical model that is being solved (see figure 1 for an example of the Maxwell model explanation), and the parameters that can be change (see figure 2)
- A 1.3 MB heavy folder containing all the necessary functions (conveniently commented) and files to perform the inverse analysis

Below, some examples that can be obtained with this code will be shown. This could be the result of tests performed by a user that would want to compare the distribution of forces in the *Drosophila melanogaster* embryo development, assuming that the tissue can be modelled using a purely viscous Kelvin-Voigt model. First case corresponds to the assumption of contractile dipoles in the edges of the numerical elements. Second case corresponds to the substitution of contractile dipoles by contractile radial and tangential pressures. Last case corresponds to a collapsed version of the second, using the same value of pressure per 5 elements (corresponding to a cellular group in the real tissue).

3.1 Examples

We can see how the user can easily extract some conclusions: Collapsing the elements, in case of contractile pressures (case 3 vs case 2) leads to a loss in accuracy quite important: contractile forces (blue if contracting pressure, red if expanding pressures) are located at the boundaries of the domain (the so called apical and basal regions), which are the areas where the highest strains are located, making it all compliant with the principles of mechanics. But, if we collapsed the elements, assuming that all those regions of the domain are under

2.2.2 Maxwell model

If now we have a system of elastic spring and viscous dashpot in series (see figure 2.2.2) the equations change, as now it is the stress what is constant for every element, $\boldsymbol{\sigma}^e = \boldsymbol{\sigma}^v = \boldsymbol{\sigma}$. The equilibrium equation that results is

$$\dot{\boldsymbol{\epsilon}} = \dot{\boldsymbol{\epsilon}}^e + \dot{\boldsymbol{\epsilon}}^v = \mathbf{D}^{-1}\dot{\boldsymbol{\sigma}} + \eta^{-1}\boldsymbol{\sigma} \tag{2.14}$$

Time discretization

If we perform the same time discretization that we did before, we get

$$\frac{\boldsymbol{\epsilon}_{n+1} - \boldsymbol{\epsilon}_n}{h} = \mathbf{D}^{-1}\frac{\boldsymbol{\sigma}_{n+1} - \boldsymbol{\sigma}_n}{h} + \eta^{-1}\boldsymbol{\sigma}_{n+\theta} \tag{2.15}$$

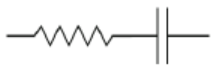

Figure 2.2: Maxwell scheme: dashpot and spring in series

Premultiplying the previous equation by elastic and viscous constitutive matrices $\mathbf{D}$ and $\boldsymbol{\eta}$:

$$\begin{aligned}
&\frac{\eta}{h}(\boldsymbol{\sigma}_{n+1} - \boldsymbol{\sigma}_n) + \mathbf{D}\boldsymbol{\sigma}_{n+\theta} = \frac{\eta\mathbf{D}}{h}(\boldsymbol{\epsilon}_{n+1} - \boldsymbol{\epsilon}_n) \implies \\
&\eta(\boldsymbol{\sigma}_{n+1} - \boldsymbol{\sigma}_n) + h\mathbf{D}((1-\theta)\boldsymbol{\sigma}_n + \theta\boldsymbol{\sigma}_{n+1}) = \eta\mathbf{D}(\boldsymbol{\epsilon}_{n+1} - \boldsymbol{\epsilon}_n) \implies \\
&(\eta\mathbf{I} + h\mathbf{D}\theta)\boldsymbol{\sigma}_{n+1} = \eta\mathbf{D}\boldsymbol{\epsilon}_{n+1} + (\eta\mathbf{I} - h\mathbf{D}(1-\theta))\boldsymbol{\sigma}_n - \eta\mathbf{D}\boldsymbol{\epsilon}_n \implies \\
&(\mathbf{I} + \frac{h}{\eta}\mathbf{D}\theta)\boldsymbol{\sigma}_{n+1} = \mathbf{D}\boldsymbol{\epsilon}_{n+1} + (\mathbf{I} - \frac{h}{\eta}\mathbf{D}(1-\theta))\boldsymbol{\sigma}_n - \mathbf{D}\boldsymbol{\epsilon}_n
\end{aligned} \tag{2.16}$$

Figure 1: Extract of the User Guide detailing the equations derived from the Maxwell viscoelastic model

```
dt=45; E = 1e-9; eta = 0.89;
macronx = 1; macrony = 5;
p = yes; px = no; py = no; cn = no;
lambdap = 0.01 ;lambdap_x =0.010; lambdacn = 0.0001; lambdap_y = 0.0001;
vmodel = Kelvin;
dim = 3;
collapsed = 0;
END

% macronx and macrony: Number of elements that make a macroelement
% p, px, py, cn = yes : if we want to have that force as OUTPUT
% p, px, py, cn = no :  if we do not want to have that force in the analysis
% p, px, py, cn = # : if we want that forces as INPUT with value #
% COLLAPSED: 1 for uncollapsed, 2 for macroelements with single value;
```

Figure 2: Extract of setup.txt, where the user can modify the values of the parameters at their will

the same contractile pressure-like forces, we would be forcing the elements that are under expansion forces to contract. At the same time, contractile pressures can be considered as similar to contractile dipoles (red if contractile, blue if expansive), but they are less mesh dependant, as they act through the whole element and not on specific edges. This actually can be assessed in comparing case 1 lowest elements to case 2 left image (radial contractile pressures). The mesh dependency on the contractile dipoles ties the set of forces to the edges, something that the contractile pressure do not suffer. This allows the contractile radial pressure to show that those lowest elements are expanding their volume, something that is lost when we assumen only forces at the edges.

4 Conclusions

The objectives were achieved, as the final code is fast, flexible to several parameters and easy to understand. Because computations for the *Drosophila* embryo case (those for which the tool was implemented) are fast, around 20 seconds for the whole integration time, tests can be carried out easily, and we can view the results and start studying them in a matter of minutes.
The further analysis of the embryo development of the *Drosophila melanogaster* is work of future researchers that will find the tool developed during this industrial training really useful. The future user does not need to know anything of Finite Element Method or linear elasticity to try and test the best set of parameters that give a (biologically speaking) satisfactory set of forces during this process, or any other, should the input mesh be different.

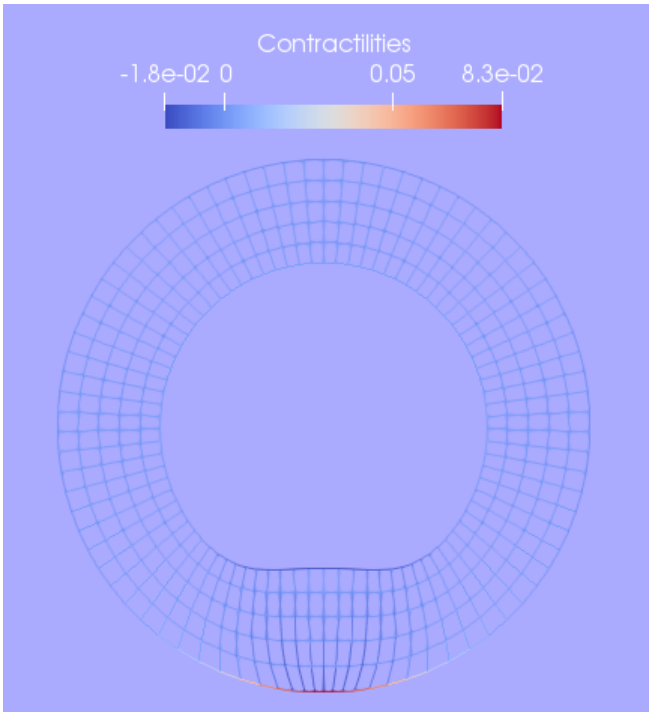

Figure 3: Step 10 of time analysis. Only contractile dipoles considered

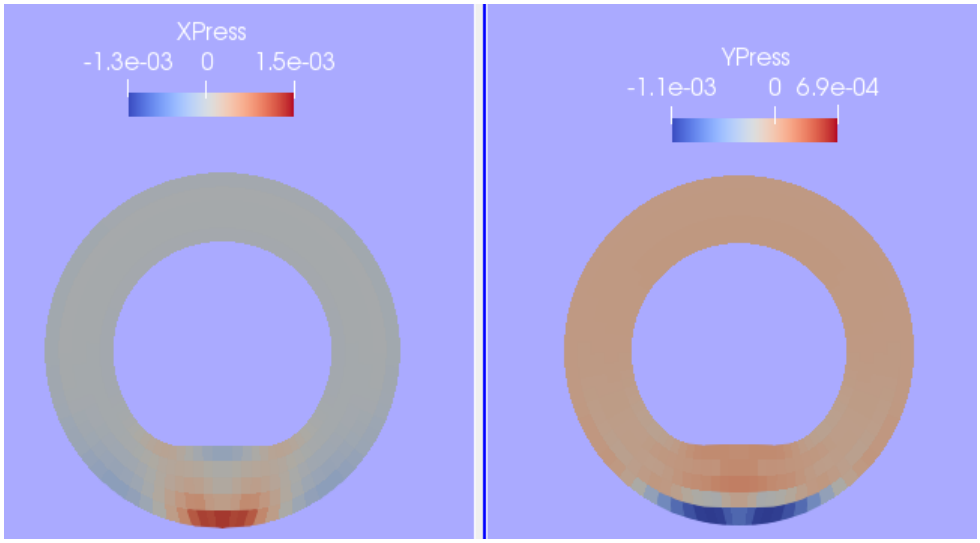

Figure 4: Step 10 of time analysis. Only contractile pressures considered

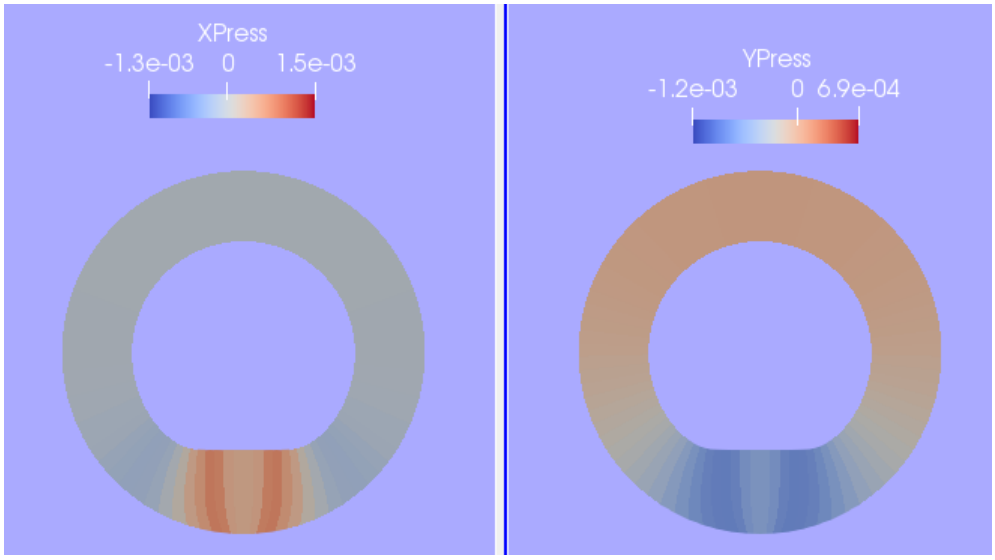

Figure 5: Step 10 of time analysis. Only contractile pressures considered, but collapsed: same values for every 5 elements in radial direction. This change only involver switching the value of *collapsed* parameter from 1 to 2