Modelling and simulation of fibrous biological tissues via discrete homogenization methods

Denis Caillerie[1], **Vuk Milišić**[2,*], **Ayman Mourad**[3], and **Annie Raoult**[4]

[1] 3S-R, UMR CNRS-UJF-INPG 5521 Domaine Universitaire, BP53 38041 Grenoble Cedex 9, France.
[2] LJK-IMAG, UMR CNRS-UJF-INPG 5523, B. P. 53, 38041 Grenoble Cedex 9, France.
[3] Université libanaise and Lebanese International University, Beyrouth, Lebanon.
[4] MAP5, Université Paris Descartes and CNRS, 45 rue des Saints Pères, 75270 Paris Cedex 06, France.

Thanks to their geometrical organization at the cell level, soft biological tissues can be modelled from the mechanical point of view as multidimensional networks of elastic bars. The length of the bars is supposed to be small with respect to the size of the macroscopic medium. We introduce a detailed description of the overall structure accounting both for the tensions due to the bars and for the moments between pairs of bars. Using quasi-periodicity hypotheses, we apply a discrete homogenization technique, [1]. We derive a continuous homogenized mechanical law in the large transformation setting. We describe the basic principles of this approach that was first introduced in the cardiac modelling context in [2]. In a last step we present its implementation in a finite element framework. We comment some aspects of our numerical results.

1 Introduction

We are interested in the mechanical behavior of muscles under external load. Such living tissues are characterized by the presence of structures with separate scales that confer to them anisotropic features. While the skeleton muscles present quite trivial fiber orientation (aligned with the bones), some organs – the heart muscle for instance – do not. In this particular case, the specific geometrical distribution of fibers inside the myocardium is still under investigation [3, 4]. From the modelling point of view, mechanical elastic energy densities are often derived empirically and "tuned" via macroscopic measures [5]. In most of them the anisotropy resulting from the fibers is taken into account. We present here a first attempt in infering the constitutive myocardium modelling from the cell level. The tissue is seen as a discrete network. Each bar in the net stands for a cell that is a constitutive contractile part of a fiber that, in turn, is a constitutive part of the muscle. In this way a description of the mechanical behavior of a single myocyte or of adjacent myocytes, when experimentally available, will be sufficient to provide a macroscopic mechanical description of the whole ventricle. In the first section of this paper we introduce the discrete network and we derive the homogenized continuous macroscopic system obtained – roughly speaking – by letting the bar length go to 0. We introduce the finite element discretization of the problem in the large deformation context. The structure of the homogenized law, which is an implicit law, requires the use of numerical procedures at the cell level. We end by commenting some numerical results in 3D obtained by a home-made development of the software *Continu* [6].

2 Discrete muti-scale homogenization

Let a network with nodes (*resp.* bars) labelled by a set $\mathcal{N}$ (*resp.* $\mathcal{B}$) be given. Let $\mathbf{R} : \mathcal{N} \mapsto \mathbb{R}^d$ be the position of its nodes under the action of loads $\mathbf{f}$ applied on the nodes. As bars remain straight, the overall position of the lattice is then known. We write down the balance of forces at each node $\tilde{n}$ and the balance of moments for each bar $\tilde{b}$. Then we put these equations under a weak discrete form by multiplying the force equations (*resp.* moment equations) by virtual discrete displacements $\mathbf{v}$, (*resp.* by virtual rotations), and by summing over nodes and bars. This leads to the following discrete virtual power formulation:

$$\sum_{\tilde{b}\in\mathcal{B}} N^{\tilde{b}}\mathbf{B}^{\tilde{b}}\cdot\Delta\mathbf{v}^{\tilde{b}} + \sum_{\tilde{c}\in\mathcal{C}} M^{\tilde{c}}\left[A^{P(\tilde{c})}\mathbf{B}^{D(\tilde{c})}\cdot\Delta\mathbf{v}^{P(\tilde{c})} + A^{D(\tilde{c})}\mathbf{B}^{P(\tilde{c})}\cdot\Delta\mathbf{v}^{D(\tilde{c})}\right] + \sum_{\tilde{n}\in\mathcal{N}}\mathbf{f}(\tilde{n})\cdot\mathbf{v}(\tilde{n}) = 0$$

where, in the first term, $\mathbf{B}^{\tilde{b}} = \mathbf{R}(E(\tilde{b})) - \mathbf{R}(O(\tilde{b}))$ is the deformed position of the bar $\tilde{b}$ with origin node $O(\tilde{b})$ and end node $E(\tilde{b})$, $\Delta\mathbf{v}^{\tilde{b}} = \mathbf{v}(O(\tilde{b})) - \mathbf{v}(E(\tilde{b}))$, and $N^{\tilde{b}}$ is the axial tension in bar $\tilde{b}$ divided by the deformed bar length. From the objectivity principle, we know that $N^{\tilde{b}}$ reduces to a function of the bar length. In the second term, $\mathcal{C}$ numbers the bar interactions, $M^{\tilde{c}}$ is the quotient of the modulus of the moment vector between two interacting bars $P(\tilde{c})$ and $D(\tilde{c})$ (which, from the objectivity principle, depends only on the scalar product of the unit vectors of the bars in their deformed position) by the product of their lengths. Finally, $A^{\tilde{b}} = \mathbf{e}^{\tilde{b}}\otimes\mathbf{e}^{\tilde{b}} - Id$ where $\mathbf{e}^{\tilde{b}} = \mathbf{B}^{\tilde{b}}/\|\mathbf{B}^{\tilde{b}}\|$. Now we suppose that the network of bars is periodic: it is obtained by the repetition of a reference pattern consisting of a finite number of nodes and bars. In the global network, each node can

* Corresponding author E-mail: vuk.milisic@imag.fr, Phone: + 33 476635738 Fax: + 33 476631263

be labelled by an index $\nu \in \mathbb{Z}^d$ that numbers the repeated pattern the node belongs to and by a local coordinate $n \in \mathcal{B}_\mathcal{R}$ that numbers the node inside this repeated cell. Similar descriptions apply to bars and bar interactions. For instance, $b \in \mathcal{B}_\mathcal{R}$ counts the number of bars in the elementary pattern. We let the bar length ϵ go to 0 and we perform an asymptotic expansion of the node positions. The claimed expansions depend on the index $n \in \mathcal{N}_\mathcal{R}$, they infer expansions on the vectors $\mathbf{B}^{\tilde{b}}$ and altogether give the usual cascade of equations in the homogenization context. We denote by λ the slow variable $\epsilon\nu$, see [1].

The zeroth order terms in ϵ imply that the zeroth order terms of the positions do not depend on the fast variable n. The first order term provides the microscopic cell problem which remains discrete and reads

$$\sum_{b\in\mathcal{B}_\mathcal{R}} N^b\mathbf{B}^b\cdot\Delta\mathbf{v}^b + \sum_{c\in\mathcal{C}_\mathcal{R}} M^c\left[A^P\mathbf{B}^D\cdot\Delta\mathbf{v}^P + A^D\mathbf{B}^P\cdot\Delta\mathbf{v}^D\right] = 0, \text{ where } \mathbf{B}^b = \Delta\mathbf{R}_1^b + \nabla_\lambda\mathbf{R}_0\delta^b, \tag{1}$$

and δ^b are vectors with integer entries related to the numbering of bars connecting distinct cells. We summarize this equation under the form $\mu(\mathbf{R}_1, \partial_\lambda\mathbf{R}_0)= 0$. It is an implicit equation that provides the increments of $\mathbf{R}_1$ in terms of the gradient of $\mathbf{R}_0$. Note that the redefinition of $\mathbf{B}^b$ comes from the first order asymptotic expansion and is typical of homogenization Anzats. The second order terms in ϵ provide the macroscopic continuous equation that reads:

$$\int_{\mathbb{R}^d}\mathbf{S}\cdot\nabla_\lambda\mathbf{v}d\lambda = \int_{\mathbb{R}^d}\mathbf{f}\cdot\mathbf{v}\,d\lambda, \text{ where } \mathbf{S} = \sum_{b\in\mathcal{B}_\mathcal{R}} N^b\mathbf{B}^b\otimes\delta^b + \sum_{c\in\mathcal{C}_\mathcal{R}} M^c\left[A^P\mathbf{B}^D\otimes\delta^P + A^D\mathbf{B}^P\otimes\delta^D\right]. \tag{2}$$

The nonlinear homogenization process contains two steps; given a macroscopic strain gradient $\partial_\lambda\mathbf{R}_0$ one solves (1) in order to define $\mathbf{R}_1$ at each point of $\mathbb{R}^d$, this is then used in order to compute the stress tensor $\mathbf{S}$ on the macroscopic scale by solving (2).

3 FEM Multi-scale Newton method

Both the micro and the macro equations are nonlinear, so that we use Newton methods at each scale in order to compute a numerical solution. In the continuous setting, there are two steps in our algorithm: set $p = 0$, then

1. at the microscopic level, at each point $\lambda \in \mathbb{R}^d$, one solves iteratively

$$\frac{\partial\mu}{\partial\mathbf{R}_1}(\mathbf{R}_1^{k+1} - \mathbf{R}_1^k) + \mu(\mathbf{R}_1^k, \nabla_\lambda\mathbf{R}_0^p) = 0, \text{ until } \sum_{n\in\mathcal{N}_\mathcal{R}} \|\mathbf{R}_1^{k+1,n} - \mathbf{R}_1^{k,n}\| < \mathrm{tol}_\mu \tag{3}$$

   for a given $\nabla_\lambda\mathbf{R}_0^p$,

2. at the macroscopic level, one performs a single resolution for a fixed p

$$\int_{\mathbb{R}^d}\frac{\partial\mathbf{S}}{\partial F}\left(\nabla_\lambda\mathbf{R}_0^{p+1} - \nabla_\lambda\mathbf{R}_0^p\right) : \nabla\mathbf{v}d\lambda + \int_{\mathbb{R}^d}\mathbf{S}(\partial_\lambda\mathbf{R}_0^p) : \nabla\mathbf{v}d\lambda = \int_{\mathbb{R}^d} f\cdot\mathbf{v}d\lambda, \text{ until } \left\|\nabla_\lambda\mathbf{R}_0^{p+1} - \nabla_\lambda\mathbf{R}_0^p\right\|_{L^2(\mathbb{R}^d)} \leq \mathrm{tol}_m$$

   where F denotes the strain gradient $\partial_\lambda\mathbf{R}_0$. Then one returns to 1 and increments p.

We discretize the problem in the finite element framework with tetrahedra and $\mathbf{P}_2$ elements. Since the application we aim at is the heart contraction, we add a pressure force imposed in the normal direction to an interior surface, this gives rise to additional nonlinear terms that participate to the linearized stiffness matrix at the macroscopic level.

4 Results & perspectives

We observe a very sensitive behavior of the multi-scale code with respect to the pressure load. The method of incremental load was necessary in order to avoid either numerical divergence or very slow convergence in the microscopic iterations. A careful analysis of the spectrum of the linearized stiffness matrices when solving (3) reveals a buckling phenomenon occurring in compression zones of the computational domain. The next step of our approach consists in studying stability issues by varying the geometry of the reference pattern and by testing several values of the underlying physical constants.

References

[1] D. Caillerie, A. Mourad, and A. Raoult, Journal of Elasticity **84**(1), 33–68 (2006).
[2] A. Mourad, Description topologique de l'architecture fibreuse et modélisation mécanique du myocarde, PhD thesis, Institut National Polytechnique, Grenoble, 2003.
[3] C. S. Peskin, Comm. Pure Appl. Math. **42**(1), 79–113 (1989).
[4] P. S. Jouk, A. Mourad, V. Milisic, G. Michalowicz, A. Raoult, D. Caillerie, and Y. Usson, European Journal of Cardio-Thoracic Surgery **31**, 916–922 (2007).
[5] D. Lin and F. Yin, ASME, J. Biomech. Eng. (1998).
[6] M. Vidrascu, Solution of non-linear elasticity problems using the Continu software, Tech. rep., INRIA-Rocquencourt, march 2001.