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Validation of a Finite Element Method framework for cardiac mechanics applications

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ABSTRACT

Modeling cardiac mechanics is a particularly challenging task, mainly because of the poor understanding of the underlying physiology, the lack of observability and the complexity of the mechanical properties of myocardial tissues. The choice of cardiac mechanic solvers, especially, implies several difficulties, notably due to the potential instability arising from the nonlinearities inherent to the large deformation framework. Furthermore, the verification of the obtained simulations is a difficult task because there is no analytic solutions for these kinds of problems. Hence, the objective of this work is to provide a quantitative verification of a cardiac mechanics implementation based on two published benchmark problems. The first problem consists in deforming a bar whereas the second problem concerns the inflation of a truncated ellipsoid-shaped ventricle, both in the steady state case. Simulations were obtained by using the finite element software GETFEM++. Results were compared to the consensus solution published by 11 groups and the proposed solutions were indistinguishable. The validation of the proposed mechanical model implementation is an important step toward the proposition of a global model of cardiac electro-mechanical activity.

Keywords: Cardiac mechanics, Finite element method, hyperelasticity, Getfem, Benchmark validation

1. INTRODUCTION

Modeling of cardiac activity is an active field of research and the state-of-art is wide and very active. Recent projects have provided interesting preliminary results towards the use of individualized, computer-based, human heart models.[1–3] Most of approaches proposed descriptions, at many different levels of detail, of the cardiac electrical activity,[4,5] the excitation-contraction coupling,[6,7] the mechanical activity[8–11] and the mechano-hydraulic coupling.[12] However, translation of these models into clinical practice remains difficult and new methodological approaches are still needed in order to bring these model-based approaches to the clinical field. The global objective of our project is to propose a model-based method for the analysis of 3D regional cardiac motion and deformation, which will be applicable to Cardiac Resynchronization Therapy (CRT) in the pre- and post-operatory phases.

In order to simulate accurately myocardial deformations, the proposed model should integrate an appropriate description of cardiac mechanics. The ventricular mechanical activity is usually described as a function of its active and passive properties. Active properties are the consequence of the shortening and lengthening of sarcomeres, which are the elementary mechanical contractile elements of myocytes. This mechanical activity is under the influence of an electrical activity, since the variation of calcium concentration during the action potential allows the development of force. Passive properties are mainly related to fiber structure and orientation, collagen properties and metabolic conditions (such as hypoxia or ischemia). This paper mainly focus on the simulation of passive mechanical properties of cardiac tissues.

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Passive myocardial properties could be described through specific mechanical constitutive laws. Most of these mechanical laws are hyperelastic, incompressible and anisotropic.[13–15] The majority of them have been determined using uniaxial (Mirsky 1976) or biaxial tension tests.[14] An empiric law based on the description of sarcomere dynamics has been proposed.[16] The simulation of these models is often based on finite element methods (FEMs).[8–11] Although this kind of formulation requires higher computational resources than other approaches, it allows a rather detailed description of the myocardium dynamics.

The implementation of FEM-based models implies several difficulties such as the definition of the constitutive law and boundary conditions, the construction of the mesh, the choice of simulation parameters that ensure stability and the validation of simulated deformations. One particular issue is the lack of analytic solutions to the problems. In this context, the use of a published benchmark[17] is a consistent way to validate and verify the accuracy of simulations. Recently, a consortium of several teams[17] provided a benchmark of three problems that require the ability to solve accurately actual features that one may come across in cardiac mechanics: pressure distribution that depends on the deformed configuration , anisotropic material properties or even active contraction of a ventricle. Such a benchmark was solved by 11 different groups and they were able to reach a consensus. The aim of this paper is to provide a validation of the first two benchmark problems by using the finite element software GETFEM++.

The rest of the paper is organized as follows. In Section 2 we introduce some preliminary material to be used in the rest of the paper. In Section 3, we formulate the mathematical model of the hyperelastic problem and provide a description of the benchmark problems we solved. Finally, in Section 4, we present numerical results and confront them with the strain given by the benchmark.

2. FINITE STRAIN ELASTICITY THEORY AND NOTATIONS

In order to introduce the concepts referred to thereafter, we recall briefly the main aspects of the theory of finite strain elasticity.

Let Ω be the reference configuration and let φ be a deformation of Ω that preserves the orientation, that is to say:

$$\varphi : \bar{\Omega} \to \Omega^{\varphi} \subset \mathbb{R}^3, \text{with } \det\nabla\varphi > 0 \text{ on } \bar{\Omega}. \tag{1}$$

Now, denote by $\boldsymbol{x}^{\varphi} = \varphi(\boldsymbol{x})$ the position of a particle $\boldsymbol{x}$ submitted to the deformation φ; the displacement field is then defined by

$$\boldsymbol{u}(\boldsymbol{x}) = \varphi(\boldsymbol{x}) - \boldsymbol{x}, \tag{2}$$

and we deduce the expression of the gradient of deformation $\boldsymbol{F}$

$$\boldsymbol{F} = \nabla\varphi = \boldsymbol{I} + \nabla\boldsymbol{u}. \tag{3}$$

To estimate the gap between a deformed configuration and a so-called rigid body motion, the Green-Lagrange strain tensor $\boldsymbol{E}$ is used

$$\boldsymbol{E} = \frac{\boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I}}{2} = \frac{1}{2}\nabla\boldsymbol{u}^T\nabla\boldsymbol{u} + \frac{1}{2}(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T). \tag{4}$$

Note that in the case of linear elasticity, supposedly too restrictive in the context of cardiac mechanics, the second order term $\frac{1}{2}\nabla\boldsymbol{u}^T\nabla\boldsymbol{u}$ is neglected.

3. MECHANICAL PROBLEMS

3.1 Mathematical model

3.1.1 Hyperelastic constitutive law

In order to take into account fiber orientation induced by the anatomical organization of cardiomyocytes, a transversally isotropic constitutive law was chosen. Its nonlinear strain energy function, the so-called Guccione's law, is given by

$$W(E) = \frac{C}{2}(e^Q - 1) \tag{5}$$

with

$$Q = b_f E_{11}^2 + b_t(E_{22}^2 + E_{33}^2 + E_{23}^2 + E_{32}^2) + b_{fs}(E_{12}^2 + E_{21}^2 + E_{13}^2 + E_{31}^2). \tag{6}$$

where E_{ij} are components of the Green-Lagrange strain tensor $\boldsymbol{E}$, defined in (4). Note that, in this configuration, the fibers are in the e_1-direction.

3.1.2 Strong formulation

We consider a hyperelastic body that occupies the bounded domain Ω, with Γ its boundary, and we denote by ν the unit outward normal on Γ. Since the body is clamped on Γ_1, the displacement field vanishes there. A volume force of density $\boldsymbol{f}_0$ acts in Ω, surface tractions of density $\boldsymbol{f}_2$ act on Γ_2.

The classical formulation of an incompressible solid in steady-state equilibrium can be stated as
Problem $\mathcal{P}$. *Find a stress field* $\boldsymbol{\Pi} : \Omega \times \mathbb{R}_+ \to \mathbb{S}^d$ *and a displacement field* $\boldsymbol{u} : \Omega \times \mathbb{R}_+ \to \mathbb{R}^d$ *such that*

$$\boldsymbol{\Pi} = \partial_{\mathbf{F}} \hat{W}(\boldsymbol{F}) \qquad \text{in} \quad \Omega, \tag{7}$$

$$\det(\mathbf{F}) = 1 \qquad \text{in} \quad \Omega, \tag{8}$$

$$\operatorname{Div} \boldsymbol{\Pi} + \boldsymbol{f}_0 = \mathbf{0} \qquad \text{in} \quad \Omega, \tag{9}$$

$$\boldsymbol{u} = \mathbf{0} \qquad \text{on} \quad \Gamma_1, \tag{10}$$

$$\boldsymbol{\Pi}\boldsymbol{\nu} = \boldsymbol{f}_2 \qquad \text{on} \quad \Gamma_2. \tag{11}$$

Now we shortly describe the physical meaning of relations (7)-(11). Equation (7) represents the generic form of a hyperelastic constitutive law where $\hat{W}(\boldsymbol{F}) = W(\boldsymbol{E})$ denote the strain energy function defined at the beginning of this section and $\boldsymbol{\Pi}$, the first Piola-Kirchhoff stress tensor. Note that by using advantageously the properties of the second Piola-Kirchhoff stress tensor $\boldsymbol{S} = \boldsymbol{F}^{-1}\boldsymbol{\Pi}$, one can prove that

$$\boldsymbol{\Pi} = \boldsymbol{F} \partial_{\mathbf{E}} W(\boldsymbol{E}). \tag{12}$$

In fact, it is a much easier to work with formulation as the strain energy function used in (5) depends explicitly on $\boldsymbol{E}$. The expression (8) describes the incompressibility condition, which means the deformation is isochoric throught the static process. Relation (9) is the equilibrium equation, where Div represents the divergence operator for tensor-valued function and $\boldsymbol{f}_0$, the density of applied volume forces. Condition (10) is the displacement boundary condition. Next, the traction boundary condition (11) states that the stress vector $\boldsymbol{\Pi}\boldsymbol{\nu}$ is given on part Γ_2 of the boundary, and is equal to the boundary force of density $\boldsymbol{f}_2$.

In fact, one has to take into account this very condition with particular care as the direction of the pressure boundary condition changes with the deformed surface orientation, and its magnitude scales with the deformed area. Therefore, if we denote by p the blood pressure, this so-called follower load expression is given by

$$\boldsymbol{f}_2 = -p \det(\boldsymbol{F}) \boldsymbol{F}^{-T} \boldsymbol{\nu}. \tag{13}$$

From now on, as prescribed in the benchmark, we assume that no volume force acts on the body.

3.2 Problems description

In what follows, we present the first two problems, as they are described in the benchmark.[17]

3.2.1 Problem 1

The first problem is the deformation of a bar in static.

- $\Omega = [0, 10 \text{ mm}] \times [0, 1 \text{ mm}] \times [0, 1 \text{ mm}]$.

- **Constitutive parameters:** Transversely isotropic, $C = 2$ kPa, $b_f = 8, b_t = 2, b_{fs} = 4$.

- **Fiber direction:** Constant along the long axis, i.e. $(1, 0, 0)$.

- **Dirichlet boundary conditions:** The left face $(x = 0)$ is fixed in all directions.

- **Pressure boundary conditions:** A pressure of 0.004 kPa is applied to the bottom face $(z = 0)$.

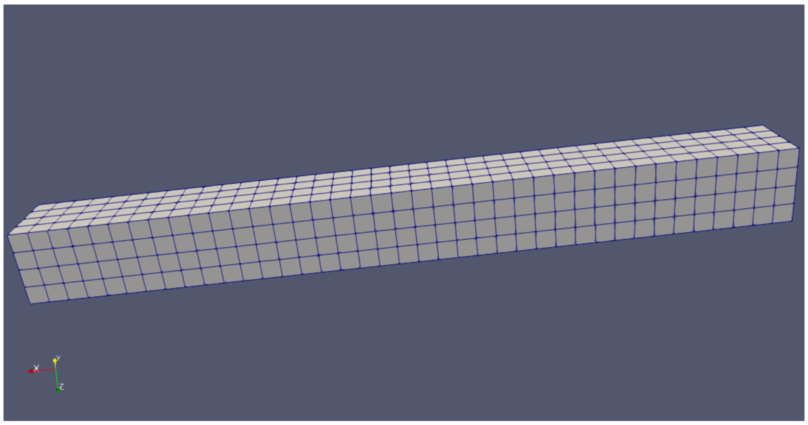

Figure 1. Reference configuration for the problem 1

3.2.2 Problem 2

Now we consider the inflation of a truncated ellipsoid-shaped ventricle whose parametrization in the undeformed configuration is given below

$$\mathbf{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} r_s \sin u \cos v \\ r_s \sin u \sin v \\ r_l \cos u \end{pmatrix} \tag{14}$$

- The undeformed geometry is defined by the volume between:
  - The *endocardial surface* $r_s = 7$ mm, $r_l = 17$ mm, $u \in [-\pi, -\arccos \frac{5}{17}], v \in [-\pi, \pi]$,
  - The *epicardial surface* $r_s = 10$ mm, $r_l = 20$ mm, $u \in [-\pi, -\arccos \frac{5}{20}], v \in [-\pi, \pi]$
  - The *base plane* $z = 5$ mm which is implicitly defined by the ranges for u.

- **Constitutive parameters:** Isotropic, $C = 10$ kPa, $b_f = b_t = b_{fs} = 1$.

- **Dirichlet boundary conditions:** The base plane $(z = 5\ mm)$ is fixed in all directions.

- **Pressure boundary conditions:** A pressure of 10 kPa is applied to the endocardium.

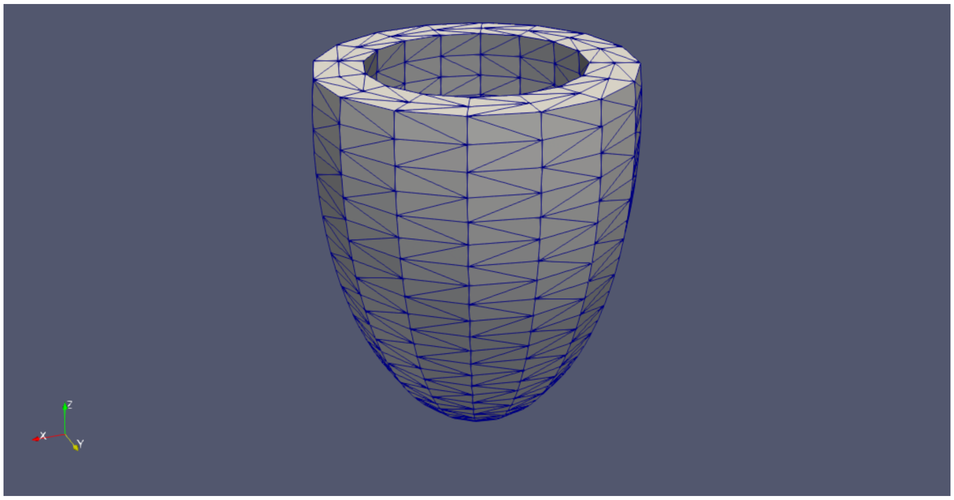

Figure 2. Reference configuration for the problem 2

3.3 Numerical methods and stability issues

As stated explicitly in the benchmark, there is no requirement regarding the computational method used to solve the problem. Here, a generalized Newton's method is used to deal with the nonlinearities arising from the hyperelastic constitutive law and the Lagrangian method was considered to enforce the incompressibility condition.

Such an approach leads to the following strain energy function

$$W_{Lag} = W(\boldsymbol{E}) - p(\det(\boldsymbol{F}) - 1) \quad \text{with } \det(\boldsymbol{F}) = 1, \tag{15}$$

with p the hydrostatic pressure. Nevertheless, to anticipate stability issues reported by several groups,[17] we still followed the suggestions of another article[18] and implemented the stabilized version of a strain energy function independent of changes in volume. In order to do so, we introduce the isochoric component of the deformation gradient

$$\bar{\boldsymbol{F}} = \det(\boldsymbol{F})^{-1/3}\boldsymbol{F}, \tag{16}$$

which by definition is such that $\det(\bar{\boldsymbol{F}}) = 1$ and we deduce that

$$\bar{\boldsymbol{E}} = \frac{\bar{\boldsymbol{F}}^T\bar{\boldsymbol{F}} - \boldsymbol{I}}{2} = \det(\boldsymbol{F})^{-2/3}\boldsymbol{E} + (\det(\boldsymbol{F})^{-2/3} - 1)\frac{\boldsymbol{I}}{2}. \tag{17}$$

Then, the expression of the new strain energy is

$$W_{iso}^{stab} = W(\bar{\boldsymbol{E}}) - p(\det(\boldsymbol{F}) - 1) + \frac{\kappa}{2}(\det(\boldsymbol{F}) - 1)^2 \quad \text{with } \det(\boldsymbol{F}) = 1. \tag{18}$$

The last term of (18) plays the role of a higher order incompressibility penalty term and is supposed to enforce more accurately the incompressibility constraint and avoid to some extent the pathological cases[19] (non-physical and unstable) where $\det(\boldsymbol{F}) < 0$.

3.4 Evaluation of the simulation

In order to evaluate the accuracy of our results, we recall here the definition of the norms used thereafter. Let $\boldsymbol{u}$ be a vector of size N, we have

$$\|\boldsymbol{u}\|_2 = \sqrt{\sum_{i=1}^{N} \boldsymbol{u}(i)^2} \tag{19}$$

$$\|\boldsymbol{u}\|_\infty = \max_i |\boldsymbol{u}(i)|. \tag{20}$$

For the second problem, we also provide the positions of the endocardial and epicardial apex, before the deformation, and the position interval obtained by the different teams, after the inflation of the ventricle. It will be used later on as one of the criteria to assess the validity of our solution.

Table 1. Position of the apex before and after the deformation.

	Endocardial apex	Epicardial apex
Reference position	$(0, 0, -17$ mm$)$	$(0, 0, -20$ mm$)$
Deformed configuration $(-z)$	25 mm (one group) $26 - 27$ mm	$27.75 - 28.75$ mm

4. RESULTS

The aim of this Section is to provide numerical simulations in order to validate the results. Note that the different numerical methods have been implemented in a code which is based on Finite Element Library in C++ under the GNU Public license: GEneric Tools for Finite Elements Methods (GETFEM++) developed by Julien Pommier and Yves Renard. For more details, we refer to http://download.gna.org/getfem/html/homepage/.

4.1 Problem 1

For the computation, we used the Augmented Lagrangian method, which require the strain energy provided in (15). We computed the solution with hexahedral elements $Q2$ for the displacement and $Q1$ for the multipliers which correspond to a problem of 20197 degrees of freedom (with a single load step) in 1012 CPU time (in seconds) on a computer with Intel Quad core processors (2.8 GHz).

In Figure 1 we plot the deformed bar; just like in the benchmark the reference solution and the computed solution are indistinguishable. To evaluate and analyse our result, we resort to the difference between our solution and the reference solution obtained for the exact same mesh (Table 2). It shows the solution is accurate enough.

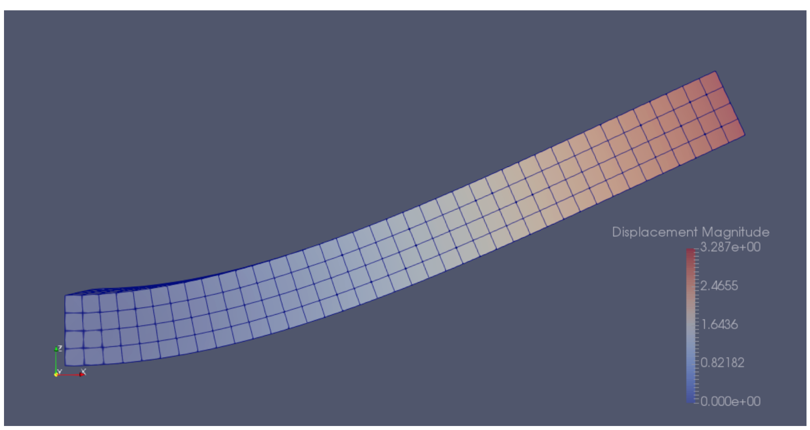

Figure 3. Superposition of the deformed configuration computed for the problem 1 and the reference solution given by the benchmark

Table 2. Accuracy of the solution with respect to the reference solution for the problem 1.

$\|\boldsymbol{u}^{ref} - \boldsymbol{u}^{getfem}\|_2$	$\|\boldsymbol{u}^{ref} - \boldsymbol{u}^{getfem}\|_\infty$
$7\ 10^{-3}$ mm	$4.8\ 10^{-2}$ mm

4.2 Problem 2

For the computation, we used the isochoric stabilized version, which require the strain energy provided in (18). We computed the solution with tetrahedral elements $P2$ for the displacement and $P1$ for the multipliers which correspond to a problem of 41984 degrees of freedom (with 25 load steps) in 1720 CPU time (in seconds) on a computer with Intel Quad core processors (2.8 GHz).

In Figure 4 we plot the inflated ventricle; just like in the benchmark the reference solution and the computed solution are still hardly distinguishable which is why we provide the difference in norm (Table 3).

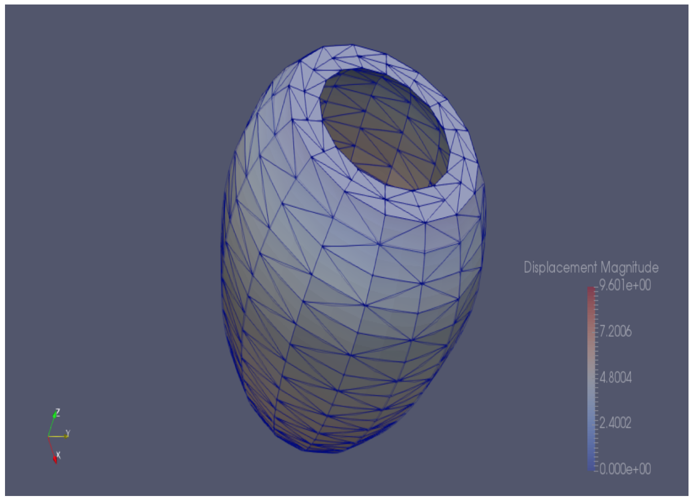

Figure 4. Superposition of the deformed configuration computed for the problem 2 and the reference solution given by the benchmark

Table 3. Accuracy of the solution with respect to the reference solution for the problem 2.

$\Vert\boldsymbol{u}^{ref} - \boldsymbol{u}^{getfem}\Vert_2$	$\Vert\boldsymbol{u}^{ref} - \boldsymbol{u}^{getfem}\Vert_\infty$
4.29 mm	0.43 mm

While we can not deny the results are not as good as in the first problem, the discrepancy among the teams also seems to be enhanced in this very case. Finally, we give in Table 4 the z-coordinate of the endocardial apex and epicardial apex after the inflation.

Table 4. Z-Position of the endocardial apex and epicardial given by Getfem in absolute value.

Endocardial apex	Epicardial apex
26.59 mm	28.26 mm

One can easily confirm in Table 1 that the obtained value are in an acceptable range in comparison with the other groups who took part in this benchmark.[17]

5. CONCLUSION

This study presented a validation of cardiac mechanics implementation, based on two benchmark problems. The results, obtained by using the finite element software GETFEM++, were compared to consensus solutions, provided by a consortium of 11 groups. In terms of three-dimensional deformation as visualized for the 2 problems, the proposed solutions are indistinguishable and the computed errors show only slight differences. The validation of the 2 problems implementation is an important step in the process of proposing a global model of cardiac mechanics. Future works will focus on the proposal of a complete model integrating electro-mechanical activations.

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