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Impact of Material Stiffness and Anisotropy on Coaptation Characteristics for Aortic Valve Cusps Reconstructed from Pericardium

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Abstract: The numerical assessment of reconstructed aortic valves competence and leaflet design optimization rely on both coaptation characteristics and the diastolic valve configuration. These characteristics can be evaluated by the shell or membrane formulations. The membrane formulation is preferable for surgical aortic valve neocuspidization planning since it is easy to solve. The results on coaptation zone sensitivity to the anisotropy of aortic leaflet material are contradictory, and there are no comparisons of coaptation characteristics based on shell and membrane models for anisotropic materials. In our study, we explore for the first time how the reduced model and anisotropy of the leaflet material affect the coaptation zone and the diastolic configuration of the aortic valve. To this end, we propose the method to mimic the real, sutured neo-leaflet, and apply our numerical shell and membrane formulations to model the aortic valve under the quasi-static diastolic pressure varying material stiffness and anisotropy directions. The shell formulation usually provides a lesser coaptation zone than the membrane formulation, especially in the central zone. The material stiffness does influence the coaptation zone: it is smaller for stiffer material. Anisotropy of the leaflet material does not affect significantly the coaptation characteristics, but can impact the deformed leaflet configuration and produce a smaller displacement.

Keywords: aortic valve; coaptation; shell; membrane; mathematical modeling; finite element method



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1. Introduction

Aortic valve disease is among the most common cardiovascular conditions that affect elderly people. According to the recent studies [1], about 4.9 million and 2.7 million elderly patients are diagnosed with aortic stenosis in Europe and North America, respectively. Y. Do et al. demonstrated that the 5 year overall survival of untreated patients with moderate aortic stenosis is only 52.3% [2]. About 28% of patients with severe aortic stenosis undergo aortic valve replacement. This corresponds to 12,129 procedures in the U.S. between 2008 and 2016 [3]. However, the estimated need for aortic valve surgery is suggested to exceed 200,000 in North America and 300,000 in Europe. In 2018, the number of procedures was increased up to 73,255 in the U.S. [4]

Cost-efficient treatment of aortic valve disease is demanded. Transcatheter aortic valve implantation (TAVI) has gained popularity and is now performed at twice the rate of the conventional surgical aortic valve replacement (SAVR) [4]. Nevertheless, SAVR remains the pivotal strategy for younger patients and concomitant surgery. According to the current guidelines, patients < 60 years old should receive mechanical prostheses, whereas patients

> 65–70 years necessitate receiving biological prostheses [5]. However, recent meta-analyses and observational studies [6–10] have considered biological prostheses to be a reasonable alternative for patients < 60 years since lifelong anticoagulation is avoided and the risk of bleeding decreases. Nevertheless, higher reoperation rates after bioprosthetic aortic valve replacement prevent its exclusive use.

In 1964, V.O. Björk and G. Hultquist reported the first results of the use of fresh autologous pericardium for aortic leaflets replacement [11]. Neo-leaflets function appeared to be poor due to their rapid calcification. J.W. Love et al. proposed to treat chemically autologous pericardium with a 0.6% glutaraldehyde solution (Carpentier's solution) [12], and the use of fixed autologous pericardium for aortic valve replacement became quite effective. Ozaki et al. established their "aortic valve neocuspidization" (AVNeo) technique based on autopericardium [13], which gained widespread interest and has become frequently performed. The authors developed their own sizers for the measurement of intercommissural distances and a template for neo-leaflets of appropriate sizes.

A recent meta-analysis by U. Benedetto et al. compared AVNeo with a number of bioprosthetic valves and the Ross procedure [14]. The authors concluded that AVNeo has a low risk of valve-related events. Moreover, AVNeo has a number of advantages: the avoidance of anticoagulation, a low transvalvular pressure gradient, an increased effective orifice area, minor regurgitation, normal aortic annulus and aortic root dimensions during cardiac cycle, low degradation and calcification, reproducibility, and a low cost [14–17].

Nevertheless, a number of drawbacks were described. As early as 1960, W.H. Muller, Jr. et al. warned not to make the neo-leaflets too large to avoid covering the coronary orifices [18]. Currently, this concern has become even more relevant, due to potential TAVI after AVNeo [19]. Moreover, it was shown that echocardiography reveals neo-leaflet thrombosis in 12.5% of patients after AVNeo [20], which is probably caused by the large surface of the neo-leaflets. To avoid these complications, one could make the neo-leaflets as small as sufficiently possible for normal aortic valve function without regurgitation. A number of criteria of normal function in the native aortic valve or after its reconstruction were described [21–25]: central coaptation height > 4 mm, effective coaptation height > 9 mm, coaptation zone above ventriculo-aortic junction, no billowing, no prolapse, and no residual regurgitation. The more the criteria are met, the better the results of the aortic valve reconstruction yielded. Numerical methods could be used for evaluating the appropriate size and shape of aortic valve neo-leaflets according to specific anatomical features of the aortic root of the particular patient in order to meet the majority of criteria of normal aortic valve function.

Optimal neo-leaflets design based on mathematical modeling is a long-standing problem in terms of bioprosthetic valve development (e.g., [26–28]) or autopericardium based neocuspidization procedure (e.g., [29]). The approaches are different in terms of the formulation for the elastic structure (membrane, shell or solid), material models used for describing the mechanical behavior of the leaflet and estimated values as a result of mathematical modeling (see review [30]). Estimated values are usually coaptation characteristics and mechanical stress in the leaflets during diastole. The coaptation characteristics indicate the valve competence and the stress associated with valve durability. In the present study, we focus on coaptation of the aortic valve under quasi-static diastolic pressure since, usually, stress fields are addressed in the literature.

Lower computational complexity makes reduced models for valve closure, such as membrane (e.g., [29,31,32] (Table 1 of [32])) or shell formulations ([32–35] (Table 1 of [32])), very popular. A leaflet optimization procedure based on the membrane formulation can be attractive in routine clinical practice, due to fast solution at the surgical planning stage. There is a promising result of using membrane formulation [29]; however, one should compare the shell and membrane formulations, taking into account the impact of the leaflet material. The first attempt was made in our preliminary study [36]: accounting for the bending stiffness reduces significantly the coaptation area for isotropic materials. However,

the shell formulation is sensitive to the initial configuration, which was not physiological in [36].

The impact of anisotropy is presented in the literature, but the results are contradictory. In [28], the authors varied the orientation of anisotropy, and for 3D solid finite element discretization, obtained insignificant changes of the coaptation area, which depends mainly on the leaflet design. A comparison of isotropic and anisotropic membrane models was carried out in [31]. According to their results, the coaptation area increases significantly in the case of anisotropic materials. However, the result is in doubt since the authors used different stress–strain curves to obtain parameter models for isotropic and anisotropic cases. Another comparison between orthotropic and isotropic shell models was presented in [37] for the pulmonary valve, which is similar to the aortic valve. Anisotropy does influence the deformed leaflet configuration, and displacement of an anisotropic leaflet is less than that of an isotropic one. Coaptation characteristics and diastolic valve configuration based on anisotropic shell and membrane models have not been compared yet.

We are interested in neocuspidization, using glutaraldehyde-treated human autopericardium. There is a lack of data on mechanical behavior on this tissue, due to the lack of a sufficient number of human samples. There is no consensus opinion on isotropy/anisotropy [38,39] and changing mechanical properties after the chemical treatment (stiffer/softer) [40,41]. Therefore, studying the impact of the leaflet material on the coaptation characteristics becomes more essential when one develops a mathematical model for the autopericardium neocuspidization procedure.

In the present paper, we study how model formulations and material stiffness/anisotropy influence the coaptation area and the deformed leaflet configuration. To this end, we apply numerical shell and membrane formulations to solve quasi-static problems of the aortic valve under diastolic pressure, varying the material stiffness and anisotropy directions. We propose a method to mimic the real, sutured neo-leaflet since shell formulation is sensitive to the initial leaflet configuration. Numerical shell formulation is based on rotation-free elements and nodal hyperelastic forces, and is thoroughly described by [36]; membrane formulation is based on nodal hyperelastic forces [42]. In the present study, we apply both formulations in the case of anisotropic material characterized by the fiber dispersion Gasser–Ogden–Holzapfel (GOH) model. The GOH model was used previously to describe native human pericardium [43] and leaflets of bioprosthetic heart valves made of glutaraldehyde-treated bovine pericardium [31,44]. Varying the parameters of the GOH model, such as the fiber dispersion, shear modulus and mean fiber direction, we consider different anisotropic and isotropic materials.

Numerical simulation is a widely used tool for design leaflet optimization, and it is useful at the surgical planning stage. That is why reduced models are preferable, but it is necessary to estimate how the model formulation influences the calculated coaptation characteristics. At the same time, the treated autopericardium seems to be efficient material for new aortic leaflets but its mechanical properties are still under investigation. In our study, we want to scrutinize how the reduced (shell/membrane) model and the leaflet material affects the coaptation zone and the diastolic configuration of the aortic valve. The results of such sensitivity analyses are important to develop the technology of aortic valve neocuspidization based on mathematical modeling.

The paper is organized as follows. We introduce parameterization of the leaflet geometry and describe our method in Section 2. In Section 3, we study the sensitivity of coaptation characteristics to the model formulation and material stiffness and anisotropy. In Section 4, we discuss our results and future work.

2. Materials and Methods

2.1. Geometry of Leaflet Design

The aortic leaflet has an attachment edge, or suturing line, which sutures the cusps to the aortic root, and a free edge, which coapts with adjacent cusps. The initial configuration of the sutured leaflet is produced by the following stages (Figure 1).

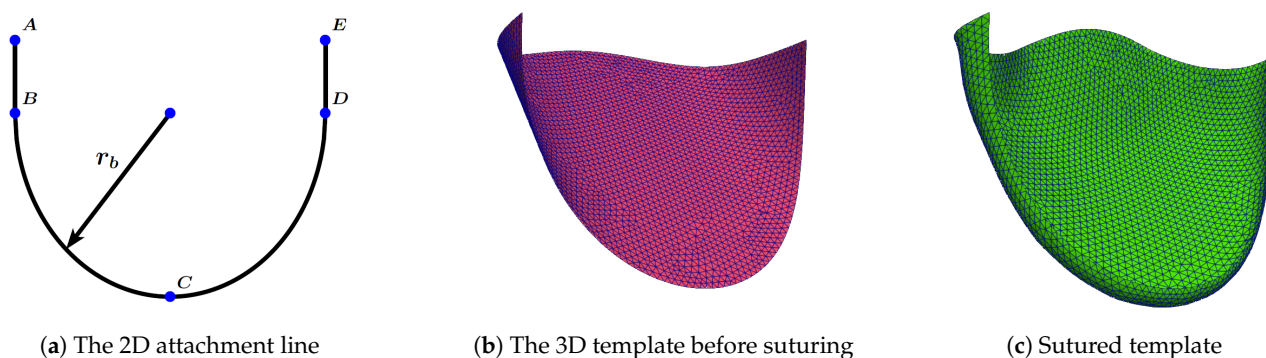


Figure 1. Pipeline for constructing sutured leaflet.

1. We define the leaflet attachment line as a curve on a plane, using four geometric parameters R , ϕ , H_c , H_b (Figure 2), where H_c is the height of the commissures, $H_b + H_c$ is the leaflet height, R is the radius of the base and the commissures (cylinder), and ϕ characterizes the angle between the surfaces of the two neighboring leaflets.

The line is defined by the following function:

$$\mathbf{r}_b(t) = (x_b(t), y_b(t)) = \begin{cases} \left(-\frac{l}{2}, H_c(1-t)\right), t \in [0;1] \\ \left(\frac{l}{2} \sin \frac{\pi(t-2)}{2}, -H_b \cos \frac{\pi(t-2)}{2}\right), t \in (1;3) \\ \left(\frac{l}{2}, H_c(t-3)\right), t \in [3;4] \end{cases} \quad (1)$$

where $l = R\phi$. Thus, the attachment line on a plane consists of two straight line segments AB and DE of length H_c and a part of ellipse BCD .

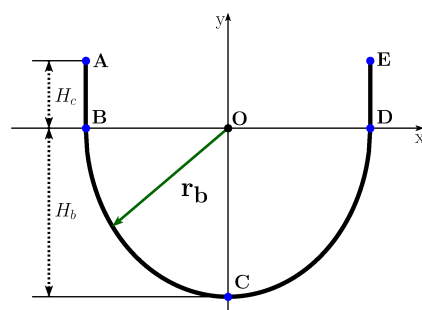


Figure 2. Attachment line on a plane.

2. We construct the 3D attachment line (in 3D space) by mapping the curve on a plane (1) to a circular cylinder of radius R (Figure 3),

$$\mathbf{r}_c(t) = (x_c(t), y_c(t), z_c(t)) = \begin{cases} x_c(t) = R \cos(x_b(t)/R), \\ y_c(t) = R \sin(x_b(t)/R), \\ z_c(t) = y_b(t). \end{cases} \quad (2)$$

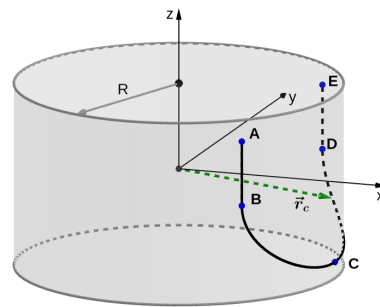


Figure 3. Attachment line on a cylinder.

3. We form the 3D leaflet template by extruding a vector $\mathbf{v}$ along the 3D attachment line (Figure 4). The direction of the vector $\mathbf{v}$ is given by an angle ω , $\mathbf{v} = (\sin \omega, 0, \cos \omega)^T$. The template surface $\Omega_{template}$ is the union of line segments started at points $\mathbf{r}_c(t)$ (2) with length

$$d(t) = \frac{H_c - z_c(t)}{\cos \omega} \cdot \{0.8 + 0.15 \cdot b(t - 2, 1, 0.5)\}, \quad b(t, t_m, w) = \frac{e^{-(t/w)^2} - e^{-(t_m/w)^2}}{1 - e^{-(t_m/w)^2}}. \quad (3)$$

Thus each point $\mathbf{x}$ of $\Omega_{template}$ may be associated with two parameters: $t, \hat{t} = (\mathbf{x} - \mathbf{A}, \mathbf{v})$.

In order to define fiber directions on the leaflet, we map the 3D surface $\Omega_{template}$ to the unfolded template $\Omega'_{template}$ on the plane $\mathcal{P}$ passing through the point $\mathbf{A} = \mathbf{r}_c(t = 0)$ with normal $\mathbf{v}$. Any point $\mathbf{x} \in \Omega_{template}$ with parameters $(t, \hat{t})$ is mapped to $\mathbf{x}' \in \Omega'_{template}$ with coordinates $(t, \hat{t})$.

4. We suture the 3D template and obtain its more realistic initial configuration by solving an auxiliary problem on the leaflet deformation (Figure 1c). For details, we refer to Section 3.1. The initial configuration mimics the sutured leaflets during neocuspidization procedure.

Thus five geometric parameters are utilized to define the initial leaflet geometry: R, ϕ, H_c, H_b and ω .

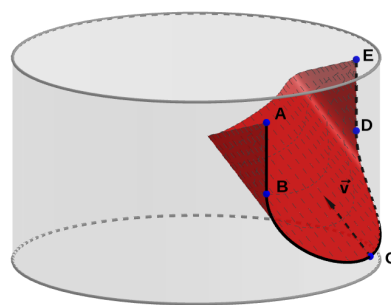


Figure 4. The 3D leaflet template before suturing.

2.2. Kinematics of Shell

We consider deformation of a thin, hyperelastic shell. We suggest that the normal to the reference mid-surface remains normal as the shell deforms (Kirchhoff–Love assumption) [45].

For compact set $\mathcal{A} \subset \mathbb{R}^2$, let mapping $\Psi : \mathcal{A} \rightarrow \Omega_0 \in \mathbb{R}^3$ describe the mid-surface for an initial configuration. A shell at the initial configuration (before deformation) $\mathcal{S}_0$ is defined as the following:

$$\mathcal{S}_0 = \{\mathbf{X} \in \mathbb{R}^3 | \mathbf{X}(\tilde{\zeta}^1, \tilde{\zeta}^2, \tilde{\zeta}^3) = \Psi(\tilde{\zeta}^1, \tilde{\zeta}^2) + \tilde{\zeta}^3 \mathbf{N}(\tilde{\zeta}^1, \tilde{\zeta}^2), \text{ where } (\tilde{\zeta}^1, \tilde{\zeta}^2) \in \mathcal{A}, \tilde{\zeta}^3 \in [-H/2, H/2]\}, \quad (4)$$

where $\mathbf{N}$ is the unit normal to the mid-surface of S_0 and H is an initial thickness of the shell. The current (deformed) configuration S_t of the shell is given by the following:

$$S_t = \{\mathbf{x} \in \mathbb{R}^3 | \mathbf{x}(\xi^1, \xi^2, \xi^3) = \boldsymbol{\psi}(\xi^1, \xi^2) + \xi^3 \lambda \mathbf{n}(\xi^1, \xi^2), \text{ where } (\xi^1, \xi^2) \in \mathcal{A}, \xi^3 \in [-H/2, H/2]\}, \quad (5)$$

where $\boldsymbol{\psi} : \mathcal{A} \rightarrow \Omega_t \in \mathbb{R}^3$ defines the mid-surface of S_t , $\mathbf{n}$ is the unit normal to the mid-surface of S_t , $\lambda = H_{def}/H$ characterizes the change in thickness, and H_{def} is the thickness of the deformed shell S_t .

The convective coordinate systems for the initial and the current configurations respectively are the following:

$$\mathbf{G}_\beta = \frac{\partial \mathbf{X}}{\partial \xi^\beta} = \boldsymbol{\Psi}_{,\beta} + \xi^3 \mathbf{N}_{,\beta}, \quad \beta = 1, 2, \quad \mathbf{G}_3 = \frac{\partial \mathbf{X}}{\partial \xi^3} = \mathbf{N}, \quad (6)$$

$$\mathbf{g}_\beta = \frac{\partial \mathbf{x}}{\partial \xi^\beta} = \boldsymbol{\psi}_{,\beta} + \xi^3 (\lambda \mathbf{n})_{,\beta}, \quad \beta = 1, 2, \quad \mathbf{g}_3 = \frac{\partial \mathbf{x}}{\partial \xi^3} = \lambda \mathbf{n}. \quad (7)$$

Here and after, we denote the partial derivative $\partial f / \partial \xi^\beta$ by $f_{,\beta}$.

The geometry of the mid-surface is characterized by the metric tensor with the following components:

$$a_{\beta\gamma} = \mathbf{g}_\beta|_{\xi^3=0} \cdot \mathbf{g}_\gamma|_{\xi^3=0} = \boldsymbol{\psi}_{,\beta} \cdot \boldsymbol{\psi}_{,\gamma}, \quad \beta, \gamma = 1, 2, \quad (8)$$

and the curvature tensor with the following components:

$$\kappa_{\beta\gamma} = -\boldsymbol{\psi}_{,\beta\gamma} \cdot \mathbf{n} = \frac{1}{2} (\boldsymbol{\psi}_{,\beta} \cdot \mathbf{n}_{,\gamma} + \boldsymbol{\psi}_{,\gamma} \cdot \mathbf{n}_{,\beta}), \quad \beta, \gamma = 1, 2. \quad (9)$$

The deformation gradient $\mathbb{F}$ is defined as follows:

$$\mathbb{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \sum_{i=1}^3 \mathbf{g}_i \otimes \mathbf{G}^i, \quad (10)$$

where $\mathbf{a} \otimes \mathbf{b} \equiv \mathbf{a} \mathbf{b}^T$, $\mathbf{G}^i = \sum_{j=1}^3 (\mathbb{G}^{-1})_{ij} \mathbf{G}_j$, matrix $\mathbb{G}$ has entries $G_{ij} = \mathbf{G}_i \cdot \mathbf{G}_j$.

The right Cauchy–Green deformation tensor $\mathbb{C} = \mathbb{F}^T \mathbb{F} = \sum_{i,j=1}^3 (\mathbf{g}_i \cdot \mathbf{g}_j) \mathbf{G}^i \otimes \mathbf{G}^j$ in the theory of thin shells is reduced to the strain measure as follows [45,46]:

$$\mathbb{C} = \sum_{\beta,\gamma=1}^2 c_{\beta\gamma} \mathbf{G}^\beta \otimes \mathbf{G}^\gamma + \lambda^2 \mathbf{N} \otimes \mathbf{N}, \quad c_{\beta\gamma} = a_{\beta\gamma} + 2\lambda \xi^3 \kappa_{\beta\gamma}, \quad (11)$$

which suggest the following matrix representation with respect to basis $\{\mathbf{G}^1, \mathbf{G}^2, \mathbf{N}\}$

$$\mathbb{C} = \begin{pmatrix} c_{11} & c_{12} & 0 \\ c_{12} & c_{22} & 0 \\ 0 & 0 & C_N \end{pmatrix}.$$

Thus, the deformation tensor $\mathbb{C}$ can be split into two parts: the surface (in-plane) part $\mathbb{C}_S = \sum_{\beta,\gamma=1}^2 c_{\beta\gamma} \mathbf{G}^\beta \otimes \mathbf{G}^\gamma$ and the out-of-plane part $\mathbb{C}_N = \lambda^2 \mathbf{N} \otimes \mathbf{N}$.

2.3. Hyperelasticity

We consider hyperelastic shells for which there exists an elastic potential $W(\mathbb{C})$ such that the second Piola–Kirchhoff stress tensor $\mathbb{S}$ is defined as the following [47]:

$$\mathbb{S} = 2 \frac{\partial W}{\partial \mathbb{C}} = \sum_{i,j=1}^3 s^{ij} \mathbf{G}_i \otimes \mathbf{G}_j, \quad s^{ij} = 2 \frac{\partial W}{\partial c_{ij}}. \quad (12)$$

To describe the mechanical behavior of the shell, we use the fiber dispersion Gasser–Ogden–Holzapfel (GOH) model [48] (Equations (2.25) and (2.26)). The GOH model was used previously to describe the native human pericardium [43] and leaflets of bioprosthetic heart valves made of glutaraldehyde-treated bovine pericardium [31,44]. Its elastic potential is the following:

$$W(\mathbb{C}) = \mu/2 \left(I_1^{(3d)} - 3 \right) + \psi_{GST}^1 + \psi_{GST}^2, \quad (13)$$

$$\psi_{GST}^\alpha = \begin{cases} \frac{k_1}{2k_2} \left\{ \exp k_2 (I_{4,\alpha}^* - 1)^2 - 1 \right\}, & I_{4,\alpha}^* > 1 \\ 0, & I_{4,\alpha}^* \leq 1 \end{cases} \quad (14)$$

$$I_1^{(3d)} = \text{tr } \mathbb{C}, \quad I_2^{(3d)} = \left((\text{tr } \mathbb{C})^2 - \text{tr } \mathbb{C}^2 \right) / 2, \quad I_3^{(3d)} = \det \mathbb{C} = (\det \mathbb{F})^2, \quad (15)$$

$$I_{4,\alpha}^* = \kappa I_1^{(3d)} + (1 - 3\kappa) I_{4,\alpha}^{(3d)}, \quad I_{4,\alpha}^{(3d)} = \mathbb{C} : (\mathbf{M}_\alpha \otimes \mathbf{M}_\alpha), \quad (16)$$

where $\alpha = 1, 2$, $\mathbf{M}_\alpha$ is the unit vector of the mean fiber direction before deformation ($\mathbf{M}_\alpha, \mathbf{N}$) = 0, κ is the dispersion parameter, usually restricted to $[0, 1/3]$. By varying parameter κ , one can obtain different anisotropic ($\kappa \neq 1/3$) and isotropic ($\kappa = 1/3$) materials.

For incompressible hyperelastic shells $I_3^{(3d)} = 1$ and the surface invariants $I_1 = \text{tr } \mathbb{C}_S$, $J^2 = \det \mathbb{C}_S$, $I_{4,\alpha} = \mathbb{C}_S : (\mathbf{M}_\alpha \otimes \mathbf{M}_\alpha)$ define the 3D invariants as follows [49]:

$$I_1^{(3d)} = I_1 + J^{-2}, \quad I_2^{(3d)} = J^2 + I_1 J^{-2}, \quad I_{4,\alpha}^{(3d)} = I_{4,\alpha}, \quad \alpha = 1, 2. \quad (17)$$

and the GOH elastic potential (13) as follows:

$$W(\mathbb{C}) = \widehat{W}(I_1, J, I_{4,\alpha}) = \mu/2 (I_1 + J^{-2} - 3) + \psi_1 + \psi_2, \quad (18)$$

$$\psi_\alpha = \begin{cases} \frac{k_1}{2k_2} \left\{ \exp k_2 (I_{4,\alpha}^* - 1)^2 - 1 \right\}, & I_{4,\alpha}^* > 1 \\ 0, & I_{4,\alpha}^* \leq 1, \end{cases} \quad (19)$$

where $\alpha = 1, 2$, $I_{4,\alpha}^* = \kappa (I_1 + J^{-2}) + (1 - 3\kappa) I_{4,\alpha}$. These equations are similar to [50] (Equations (40)–(43)).

The constitutive relations for the incompressible hyperelastic shell according to (12) are in the form of the plane stress state as follows:

$$\mathbb{S} = \sum_{\alpha,\beta=1}^2 s^{\alpha\beta} \mathbf{G}_\alpha \otimes \mathbf{G}_\beta, \quad (20)$$

$$s^{\alpha\beta} = 2 \frac{\partial \widehat{W}}{\partial c_{\alpha\beta}} = 2 \left(\frac{\partial \widehat{W}}{\partial I_1} (\mathbb{G}^{-1})_{\alpha\beta} + \frac{J}{2} \frac{\partial \widehat{W}}{\partial J} (\mathbb{C}_S^{-1})_{\alpha\beta} + \sum_{\gamma=1}^2 \frac{\partial \widehat{W}}{\partial I_{4,\gamma}} (\mathbf{M}_\gamma \otimes \mathbf{M}_\gamma)_{\alpha\beta} \right), \quad (21)$$

where $(\mathbb{B})_{\alpha\beta}$ denotes $\alpha\beta$ -entry of matrix $\mathbb{B}$.

2.4. Weak Formulation

We consider the equilibrium of a thin shell under mixed boundary conditions. Let the boundary of the mid-surface $\partial\Omega_t$ be split into two parts, $\partial\Omega_t = \Gamma_u(t) \cup \Gamma_\sigma(t)$, $\Gamma_u(t) = \bar{\Gamma}_u(t)$. The boundary conditions are the following:

$$\mathbf{u} = \bar{\mathbf{w}} \quad \text{on } \Gamma_u(t), \quad \mathbb{T}\mathbf{n}_t = \bar{\mathbf{t}} \quad \text{on } \Gamma_\sigma(t), \quad (22)$$

where $\mathbf{u} = \mathbf{x} - \mathbf{X}$ is the mid-surface displacement, $\mathbf{n}_t$ is the unit outward normal to $\partial\Omega_t$, $\mathbb{T} = (1/\det \mathbb{F}) \mathbb{F} \mathbb{S} \mathbb{F}^T$ is the Cauchy stress tensor, and $\bar{\mathbf{w}}$ and $\bar{\mathbf{t}}$ are the given displacement and tension on corresponding boundaries.

For weak formulation, we use the virtual work principle [51]: find $\mathbf{u} \in \tilde{\mathbf{H}}^1(\Omega_t)$, $\tilde{\mathbf{H}}^1(\Omega_t) := \{\mathbf{v} \in (H^1(\Omega_t))^3, \mathbf{v} = \bar{\mathbf{w}} \text{ on } \Gamma_u(t)\}$ such that

$$\delta U - \delta W_{ext} = 0, \quad (23)$$

$$\delta U = \delta \left(\int_{\mathcal{S}_0} \hat{W}(I_1(\nabla \mathbf{u}), J(\nabla \mathbf{u}), I_{4,1}(\nabla \mathbf{u}), I_{4,2}(\nabla \mathbf{u})) dV \right), \quad (24)$$

$$\delta W_{ext} = \int_{\Gamma_\sigma(t)} \bar{\mathbf{t}} \cdot \delta \mathbf{u} dt + \int_{\Omega_t} \mathbf{b} \cdot \delta \mathbf{u} ds, \quad (25)$$

where $\mathbf{b}$ is the external forces density.

We can rewrite (23)–(25) taking into account (11) and (20) as follows:

$$\delta U = \int_{\Omega_0} \mathbf{l} : \delta \mathbf{a}(\nabla \mathbf{u}) ds + \int_{\Omega_0} \mathbf{m} : \delta \boldsymbol{\kappa}(\nabla \mathbf{u}) ds, \quad (26)$$

$$\mathbf{l} = (l_{11}, l_{22}, l_{12})^T, \quad l_{ij} = \int_{-H/2}^{H/2} s^{ij} d\tilde{\zeta}^3, \quad (27)$$

$$\mathbf{m} = (m_{11}, m_{22}, m_{12})^T, \quad m_{ij} = \int_{-H/2}^{H/2} s^{ij} \lambda \tilde{\zeta}^3 d\tilde{\zeta}^3, \quad (28)$$

$$\mathbf{a} = (a_{11}, a_{22}, 2a_{12})^T, \quad \boldsymbol{\kappa} = (\kappa_{11}, \kappa_{22}, 2\kappa_{12})^T. \quad (29)$$

The in-plane membrane behavior is represented by the first term in (26), whereas the bending part is characterized by the second term in (26). We use the nodal hyperelastic force method [42] to discretize the membrane part and the approach proposed by Oñate et al. [46] to discretize the bending part. Details of the method are presented in [36]; here, we recall its main constituents.

2.5. Discretization

Let the initial mid-surface configuration Ω_0 be given as a consistent triangular mesh. We apply the linear finite elements for the membrane part and the rotation-free bending elements for the shell bending part to the approximate solution of Equations (23), (25) and (26).

Let the deformation of a triangle T_P with vertices $\mathbf{P}_1, \mathbf{P}_2, \mathbf{P}_3$ into a triangle T_Q with vertices $\mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3$ be defined via mapping $\mathbf{x}(\mathbf{X})$ (see Figure 5a). We denote the areas of undeformed triangle T_P and deformed triangle T_Q by A_P and A_Q , respectively. One of the surface invariants is the Jacobian of the deformation $J = A_Q/A_P$. The unit normal to the plane of triangle T_Q is denoted by $\mathbf{n}$.

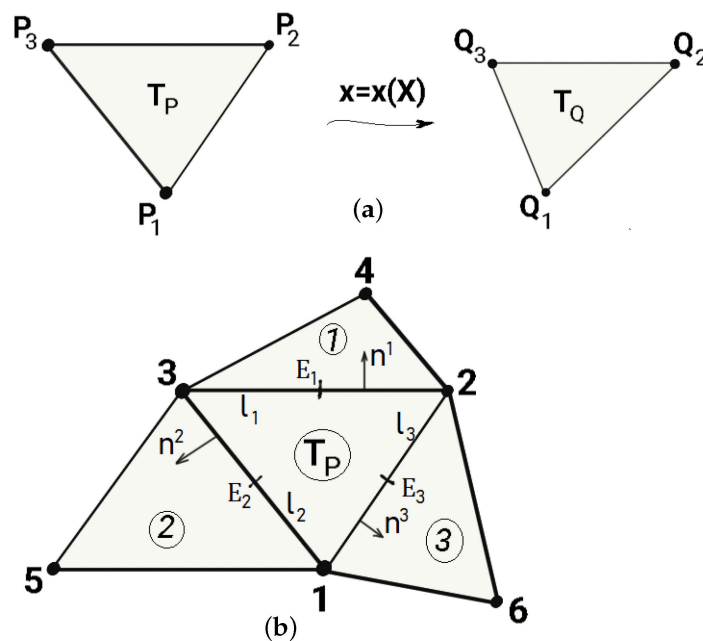


Figure 5. (a) Deformation of triangle. (b) Patch of elements consisting of the central triangle T_P and three adjacent elements. The figure from [36].

If $\mathbf{M}_\alpha^P$ is a given direction of anisotropy on the triangle T_P , this direction is mapped on triangle T_Q to the following:

$$\mathbf{M}_\alpha^Q = \frac{\mathbf{F}\mathbf{M}_\alpha^P}{\|\mathbf{F}\mathbf{M}_\alpha^P\|},$$

where $\mathbf{F}$ is the deformation gradient, which can be computed from [42] as follows:

$$\mathbf{F} = \mathbf{Q}\mathbf{D}_P^T, \quad (30)$$

and matrices $\mathbf{Q}$ and $\mathbf{D}_P$ are formed by the following vectors:

$$\mathbf{Q} = (\mathbf{Q}_1, \mathbf{Q}_2, \mathbf{Q}_3); \quad \mathbf{D}_P = (\mathbf{D}_1, \mathbf{D}_2, \mathbf{D}_3), \quad \mathbf{D}_i = \frac{1}{2A_P} \mathbf{n}_P \times (\mathbf{P}_{(i+1)\%3+1} - \mathbf{P}_{i\%3+1}), \quad (31)$$

and operator $\%3$ defines division modulo 3, and $\mathbf{n}_P$ is 3D normal to T_P .

2.5.1. Discretization of the Membrane Part

We discretize the membrane part of the deformation of T_P by the following:

$$\delta U_m^h = \int_{T_P} \mathbf{1} : \delta \mathbf{a}(\nabla \mathbf{u}^h) ds, \quad (32)$$

where $\mathbf{u}^h$ is a linear finite element displacement and the corresponding nodal force for the j -th node of triangle T_P is the following:

$$\mathbf{F}_j^m(T_P) = -\frac{\partial U_m^h}{\partial \mathbf{Q}_j} = -A_P H \frac{\partial \widehat{W}^h|_{\xi^3=0}}{\partial \mathbf{Q}_j}. \quad (33)$$

Here, the elastic potential $\widehat{W}^h|_{\xi^3=0}$ is constant over T_P since it is computed from the linear displacement $\mathbf{u}^h$.

2.5.2. Discretization of Bending Part

We discretize the bending part of the deformation of T_P by rotation-free triangular shell elements [46].

$$\delta U_b^h = \int_{T_P} \mathbf{m} : \delta \kappa (\nabla \mathbf{u}^h) ds. \quad (34)$$

The curvature tensor is obtained from nodal displacements of a patch of elements Π_P composed of the central triangle (T_P) and three adjacent triangles (Figure 5b triangles 1,2,3).

Bending forces at the i -th node of the patch Π_P are defined by the following:

$$\mathbf{F}_i^b = -A_P \frac{\delta U_b^h}{\delta \mathbf{Q}_i}, \quad i = 1, \dots, 6, \quad (35)$$

and contribution of the patch Π_P to the nodal bending forces is the following:

$$(\mathbf{F}_1^b, \mathbf{F}_2^b, \mathbf{F}_3^b, \mathbf{F}_4^b, \mathbf{F}_5^b, \mathbf{F}_6^b) = -A_P \mathbf{n} \otimes (\mathbf{m}^T \mathbf{B}_b), \quad (36)$$

where $\mathbf{B}_b$ is the curvature matrix [46] (EBST case).

2.5.3. External Forces

We introduce leaflet contact forces to prevent interpenetration of the leaflets. To reduce the computational complexity of the contact force evaluation, we add virtual contact surfaces, following [28,33].

Let $\mathcal{P}$ be a plane with outward normal $\mathbf{n}_P$ and $\mathbf{R}$ be a point on $\mathcal{P}$. For the $\mathbf{Q}_i$ node, we define the contact (collision) force as follows:

$$\mathbf{F}_{i,\text{contact}} = \frac{\eta_1 \sum_i A_i}{3} f(d) \mathbf{n}_P, \quad d = (\mathbf{Q}_i - \mathbf{R}) \cdot \mathbf{n}_P, \quad f(d) = \max\left(1 - \frac{2d}{\eta_2}, 0\right). \quad (37)$$

Here, $f(d)$ is a penalty function, coefficient η_2 characterizes the threshold distance, and coefficient η_1 characterizes the contact force value; $\sum_i A_i$ is the sum of areas of all oriented triangles sharing the $\mathbf{Q}_i$ node at the current configuration.

In order to account for the impact of leaflet suturing, at the final stage of the initial configuration search, we introduce nodal suturing forces, which orient boundary triangular elements to be tangent to the aortic surface. Let T be a boundary triangular element with vertices A, B, C , $\mathbf{e} \equiv \mathbf{x}_B - \mathbf{x}_A$ be the sutured edge, and a tangent vector $\mathbf{b} \perp \mathbf{e}$ be given (see Figure 6).

The suturing force $\mathbf{F}_{sut}$ acts only on vertex C to shift it to the position C' and rotate T to new position ABC' . Let $\mathbf{q}$ be the unit altitude vector of T and $\mathbf{n}_T$ be the unit outward normal for T . Let $\varphi_T \in [-\frac{\pi}{2}, \frac{3\pi}{2}]$ be the solution of the following system:

$$\begin{cases} \mathbf{b} \cdot \mathbf{q} = \cos \varphi_T, \\ \mathbf{b} \cdot \mathbf{n}_T = -\text{sign}(K) \sin \varphi_T, \end{cases} \quad (38)$$

where K is a suturing force parameter for $K > 0$, and φ_T is the angle between vectors $\mathbf{b}$ and $\mathbf{q}$.

The suturing force applied to vertex C (Figures 6 and 7) is defined by the following:

$$\mathbf{F}_{sut} = K f(\varphi_T) \|\mathbf{e}\| \mathbf{n}_T, \quad f(\varphi) = \begin{cases} 3 - \cos \varphi, & \varphi \in [-\frac{\pi}{2}, 0] \\ 1 + \cos \varphi, & \varphi \in [0, \pi] \\ (-\cos \varphi) - 1, & \varphi \in [\pi, \frac{3\pi}{2}] \end{cases} \quad (39)$$

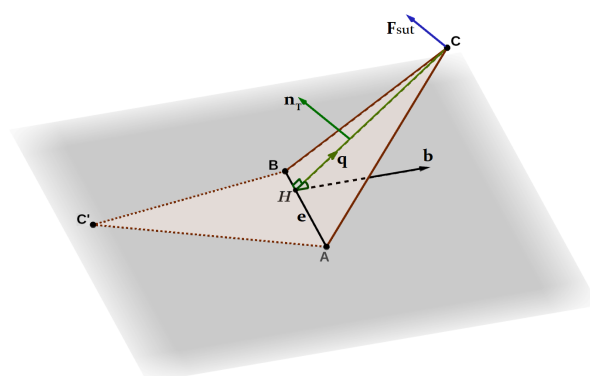


Figure 6. Sketch for defining the nodal suturing force $\mathbf{F}_{sut}$.

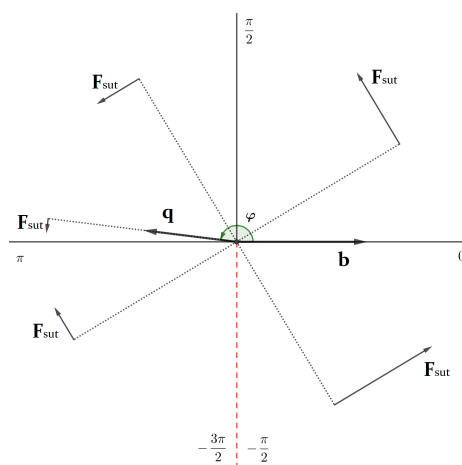


Figure 7. Dependence of the nodal suturing force $\mathbf{F}_{sut}$ on the angle φ .

2.5.4. Discretized Equilibrium Equations

The equilibrium Equations (23)–(29) form a nonlinear system for new positions $\mathbf{Q}_i$. We assemble contributions of all triangles T_P and obtain the static equilibrium for the i -th node as follows:

$$\sum_{T_P \in \Sigma_i} (\mathbf{F}_i^m(T_P) + \mathbf{F}_{i,ext}(T_P)) + \sum_{patch \in \Pi_i} \mathbf{F}_i^b = 0, \quad (40)$$

$$\mathbf{F}_{i,ext}(T_P) = \int_{\Gamma_\sigma(t) \cap T_Q} \bar{\mathbf{t}} \lambda_i ds + \int_{T_Q} \mathbf{b} \lambda_i d\mathbf{x},$$

here, Σ_i is the set of triangles sharing the i -th node, Π_i is the set of patches containing the i -th node, and λ_i are the barycentric coordinates of a material point $\mathbf{X} \in T_P$.

The nonlinear system of algebraic Equation (40) is as follows:

$$\mathcal{F}(\mathbf{Q}) = \mathbf{0}, \quad (41)$$

and is solved by combination of the inexact Newton method and relaxation method described below.

2.5.5. Computational Algorithms

A physiologically relevant initial leaflet configuration accounting suturing via suturing forces with variable coefficient K in (39) is computed by Algorithm 1. The auxiliary deformation problem is solved by the above shell finite element model, and the algebraic systems are solved by the inexact Newton method with line search from KinSol [52]. The stopping criterion for nonlinear problems is the reduction of the residual by a factor of 10^7 .

Algorithm 1 Algorithm of suturing leaflet

- 1: Set initial value of suturing force parameter $K \leftarrow 1$.
- 2: As the initial approximation, we specify the current configuration of the sutured leaflet.
- 3: **repeat**
- 4: Solve the auxiliary deformation problem with the initial approximation.
- 5: Set $K \leftarrow 2 \cdot K$
- 6: **until** $\max_T(\sin \varphi_T) < \varepsilon_{sew} = 0.01$, where maximum is searched among all sutured triangles T and the angle φ_T is given in (38)–(39).

The result of the application of Algorithm 1 is demonstrated in Figure 8. The obtained leaflet configuration after suturing (sutured configuration) is the initial configuration for finding the diastolic state of the reconstructed aortic valve. Further, we neglect all residual stresses, i.e., the initial (sutured) configuration is assumed to be stress free and load free.

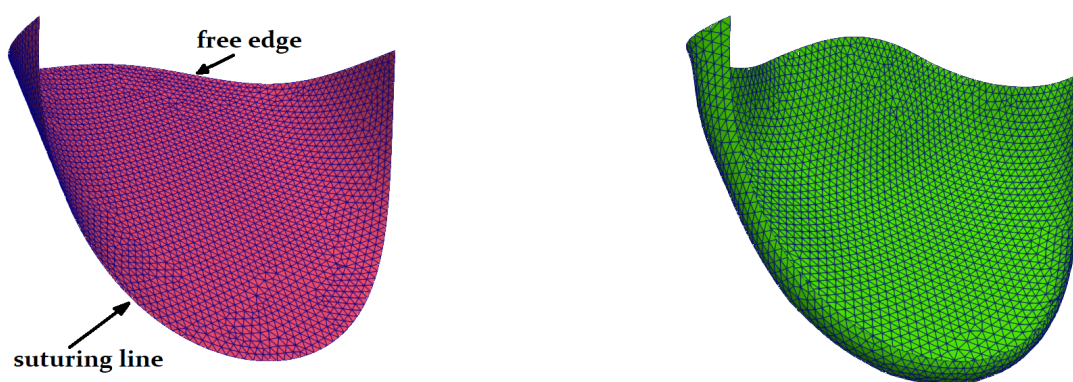


Figure 8. Initial template before suturing (left). Template after suturing (right).

To solve the system of nonlinear Equation (41), we combine the relaxation method and the Newton method (Algorithm 2) for the following reasons. The Newton method is effective for convex problems and stiff materials and fails to converge for soft materials, especially in membrane formulation. On the contrary, the relaxation method is efficient for soft materials, especially in membrane formulation and is slow for stiff materials. The combined method seeks to exploit the merits of both approaches.

Algorithm 2 Combined Newton and relaxation methods

- 1: Set the number of iteration for relaxation method N_{relax} and initial relaxation parameter $\lambda = \lambda_0$
- 2: **while** Residual norm $> 10^{-4}$ **do**
- 3: Perform N_{relax} iterations by relaxation method with varying λ
- 4: Apply the inexact Newton method until convergence or stagnation (see KinSol [52] stop conditions)
- 5: **end while**

For the Newton method, we use the inexact Newton method with the line search strategy from package Kinsol [52] with parameters $\text{FuncNormTol} = 10^{-4}$ mN, $\text{ScaledStepTol} = 10^{-5}$, $\text{MaxSetupCalls} = \text{MaxSubSetupCalls} = 1$. For solving linear system, we use the iterative solver BiCGStab with preconditioner MPT_ILUC from platform INMOST [53]. The relaxation method is described by Algorithm 3 with $\lambda_0 = 10^{-4}$ m/N for membrane and $\lambda_0 = 10^{-6}$ m/N for shell, $N_{relax} = 1000$. Note that N_{relax} should be decreased for the stiff material and increased for a soft material.

Algorithm 3 Algorithm of relaxation method

```

1: On Input: Maximal number of iteration  $N_{relax}$ , variable parameter of relaxation  $\lambda$ ,
   threshold  $\varepsilon_{abs} = 10^{-4}$ , initial guess  $\mathbf{x}^0$ , residual function  $\mathbf{f}(\mathbf{x})$ .
2: Set  $N_{bad} = 15$ ;  $r_{scl} = 0.8$ ;  $r_{bad} = 3$ 
3:  $i \leftarrow 0$ ,  $\lambda^0 = \lambda$ ,  $n_{bad} \leftarrow 0$ 
4: Compute  $R^i = \|\mathbf{f}(\mathbf{x}^i)\|$  as residual norm at the  $i$ -th iteration
5: while  $R^i > \varepsilon_{abs}$  and  $i < N_{relax}$  do ▷ Definition of 'bad' iteration are lines 5–8
6:   if  $\lambda \cdot R^i > r_{bad} \cdot \lambda^0 \cdot R^0$  then
7:      $\lambda^i \leftarrow \lambda^0 R^0 / R^i$ 
8:      $n_{bad} \leftarrow n_{bad} + 1$ 
9:   else
10:     $\lambda^i \leftarrow \lambda$ 
11:   end if
12:   if  $n_{bad} \geq N_{bad}$  then
13:      $\lambda \leftarrow r_{scl} \lambda$ 
14:      $n_{bad} \leftarrow 0$ 
15:   end if
16:    $\mathbf{x}^{i+1} = \mathbf{x}^i + \lambda^i \cdot \mathbf{f}(\mathbf{x}^i)$ 
17:    $i \leftarrow i + 1$ 
18: end while

```

3. Test Problems and Results**3.1. Setting the Problems**

In all numerical experiments, we consider the template with parameters $R = 15$ mm, $H_c = 1.5$ mm, $H_b = 15$ mm, the thickness of leaflet $H = 0.4$ mm, $\omega = -\frac{2\pi}{9}$ radians and $\phi = \frac{2\pi}{3} - 0.4$ radians, where 0.4 radians corresponds to suturing indent ([54] (Figure 2b)).

For the 3D surface $\Omega_{template}$ we generate three quasi-uniform unstructured triangular grids with mesh sizes $h_1 = 0.5$ mm, $h_2 = h_1/2$, $h_3 = h_1/4$. The comparisons of the coaptation characteristics computed on these meshes indicate that the mesh convergence is achieved on the coarse grid. All presented results correspond to the mesh size h_1 .

As with the auxiliary problem for suturing, we consider the deformation of an isotropic neo-Hookean shell with elastic potential for the shell as $\psi_{NKH} = \mu/2(I_1 + J^{-2} - 3)$ under a constant pressure of 90 mmHg, $\mu = 900$ kPa and a leaflet thickness of $H_t = 0.8$ mm. The leaflet thickness is increased in order to obtain a more smooth configuration in the vicinity of the suturing line. A homogenous Dirichlet boundary condition for displacements is applied at the suturing line. In order to avoid an undesirable initial configuration, we apply contact forces (37) at three contact (penalty) surfaces presented in Figure 9:

Plane MN: $\mathbf{n}_P = (1, 0, 0)^T$, $\mathbf{R} = (0.2R, 0, 0)^T$, $\lambda_1 = 270$ mmHg, $\lambda_2 = 0.01R$;

Plane AM: $\mathbf{n}_P = (\sin \frac{\pi}{3}, \cos \frac{\pi}{3}, 0)^T$, $\mathbf{R} = (0, 0, 0)^T$, $\lambda_1 = 360$ mmHg, $\lambda_2 = 0.01R$;

Plane NE: $\mathbf{n}_P = (-\sin \frac{\pi}{3}, \cos \frac{\pi}{3}, 0)^T$, $\mathbf{R} = (0, 0, 0)^T$, $\lambda_1 = 360$ mmHg, $\lambda_2 = 0.01R$.

The obtained by Algorithm 1 leaflet configuration after suturing (sutured configuration) is the stress-free and load-free initial configuration for finding the diastolic state of the reconstructed aortic valve.

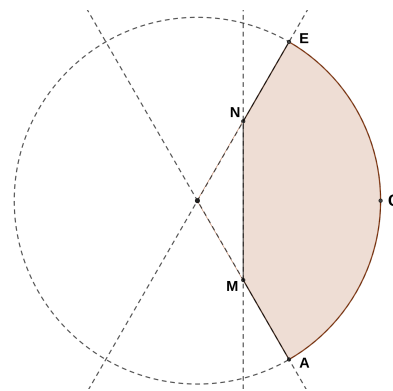


Figure 9. Schematic representation of contact (penalty) planes by segments AM , MN , and NE . The pink area is the allowed area for the sutured leaflet configuration. In fact, the cylindrical surface is not a constraint, and during the simulation, the template can freely go beyond it.

To compute the diastolic configuration of the closed aortic valve, we consider deformation of the sutured leaflet under constant diastolic pressure of $P = 90$ mmHg. The leaflet material is described by GOH model (18) with varying parameters $\mu \in \{900, 3000\}$ kPa, $k_1 = 1100$ kPa, $k_2 = 1000$, $\kappa \in \{0.2, 0.29, 1/3\}$, $\theta \in \{0, \frac{\pi}{8}, \frac{\pi}{4}, \frac{3\pi}{8}, \frac{\pi}{2}\}$, where $\mathbf{M}_1 = \cos \theta \mathbf{e}_x + \sin \theta \mathbf{e}_y$, $\mathbf{M}_2 = \cos \theta \mathbf{e}_x - \sin \theta \mathbf{e}_y$, $\mathbf{e}_x, \mathbf{e}_y$ are Cartesian vectors. Most of the model parameters are taken from [44] and correspond to the glutaraldehyde-treated bovine pericardium. (There is a lack of information on the fixed human pericardium.)

The suturing line is assumed to be clamped. The clamped boundary in shell formulation is treated, following [46]. We evaluate the curvature tensor from the condition of vanishing linearized moments in the case of close-to-boundary incomplete patches [36]. We solve the equilibrium state problems both in shell and membrane formulations.

Taking into account the symmetry of the problem, we consider the deformation of only one leaflet with two contact (penalty) planes:

Left: $\mathbf{n}_P = (\sin \frac{\pi}{3}, \cos \frac{\pi}{3}, 0)^T$, $\mathbf{R} = (0, 0, 0)^T$, $\lambda_1 = 1.1 \cdot 90$ mmHg, $\lambda_2 = 0.01R$;

Right: $\mathbf{n}_P = (-\sin \frac{\pi}{3}, \cos \frac{\pi}{3}, 0)^T$, $\mathbf{R} = (0, 0, 0)^T$, $\lambda_1 = 1.1 \cdot 90$ mmHg, $\lambda_2 = 0.01R$.

The leaflet in the initial configuration, the two contact planes, and the boundary conditions are presented in Figure 10.

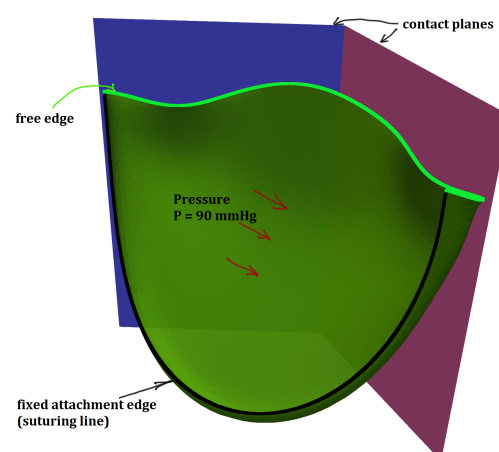


Figure 10. Boundary conditions for leaflet: left contact plane (blue); right contact plane (red); clamped attachment line (black); free edge (green).

3.2. Configuration of the Closed Valve

We study the influence of the model formulation, material stiffness and anisotropy on the deformed leaflet configuration by varying the shear modulus μ , the fiber dispersion κ and mean fiber direction θ .

The model formulation (membrane or shell) significantly influences the deformed shape (see Figures 11 and 12 for isotropic cases, and Figures 13 and 14 for anisotropic cases). In particular, displacements of the free edge and belly region are significantly smaller for the shell model.

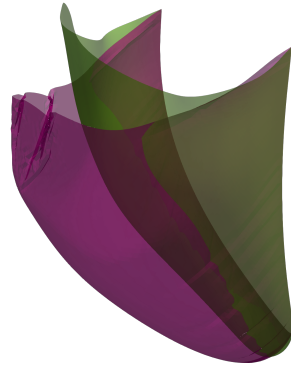


Figure 11. Isotropic, membrane, $\mu = 900$ kPa. Initial configuration (green); deformed configuration (red).



Figure 12. Isotropic, shell, $\mu = 900$ kPa. Initial configuration (green); deformed configuration (red).

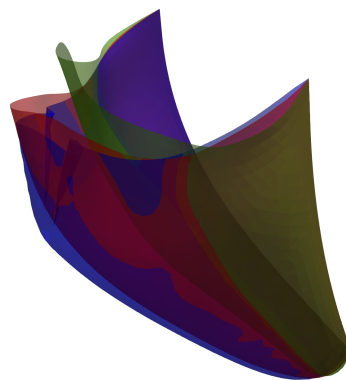


Figure 13. Anisotropic, $\mu = 900$ kPa, $\kappa = 0.2$, $\theta = 0$. Initial configuration (green); deformed shell (red); deformed membrane (blue).

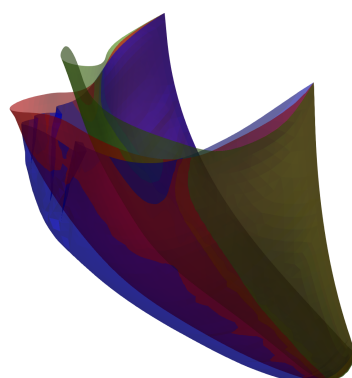


Figure 14. Anisotropic, $\mu = 3000$ kPa, $\kappa = 0.29$, $\theta = \pi/4$. Initial configuration (green); deformed shell (red); deformed membrane (blue).

The comparisons of the isotropic and anisotropic materials in the scope of one model are presented in Figures 15–18. The anisotropy influence is more prominent for soft materials, and in some cases, anisotropy leads to significantly smaller vertical displacement of the free edge and the belly region, compared to the isotropic cases (e.g., $\kappa = 0.2$, $\theta = 0$ on Figures 15 and 16). Similar conclusions are derived from the comparison of closed pulmonary valves for orthotropic and isotropic materials [37] (Figure 4c,d). However, for stiff materials ($\mu = 3000$ kPa, Figures 17 and 18), there are no significant differences between isotropic and anisotropic cases for both membrane and shell models.



Figure 15. Membrane, $\mu = 900$ kPa; isotropic (red); anisotropic $\kappa = 0.29$, $\theta = \pi/4$ (green); anisotropic $\kappa = 0.2$, $\theta = 0$ (blue).



Figure 16. Shell, $\mu = 900$ kPa; isotropic (red); anisotropic $\kappa = 0.29$, $\theta = \pi/4$ (green); anisotropic $\kappa = 0.2$, $\theta = 0$ (blue).



Figure 17. Membrane, $\mu = 3000$ kPa; isotropic (red); anisotropic $\kappa = 0.29$, $\theta = \pi/4$ (green); anisotropic $\kappa = 0.2$, $\theta = 0$ (blue).

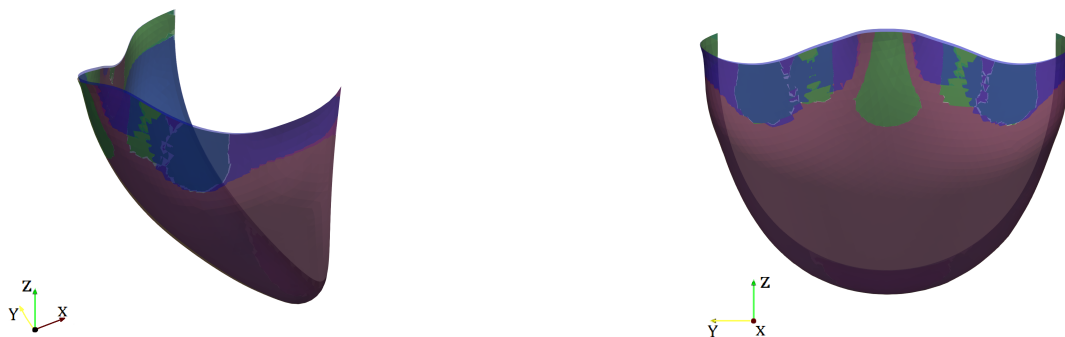


Figure 18. Shell, $\mu = 3000$ kPa; isotropic (red); anisotropic $\kappa = 0.29$, $\theta = \pi/4$ (green); anisotropic $\kappa = 0.2$, $\theta = 0$ (blue).

3.3. Coaptation Profiles and Coaptation Characteristics

In Figure 19, we present the coaptation area A_{cpt} for different model parameters and model formulations.

The coaptation zone is a set of points in the leaflet for which its sign distance to a penalty plane does not exceed $0.01R$. Both material stiffness and model formulation influence A_{cpt} : it is smaller for the shell model. However, there are no decisive trends for how it is affected by anisotropy that agrees with the observation [28] (Figure 7).

The deviation between shell and membrane models is the most prominent for a stiffer material (Figure 20); the conclusion is supported by the analysis of the coaptation profiles (Figures 21–24).

In the scope of one model formulation, the anisotropy degree (variable κ , Figures 23 and 24) and anisotropy direction (variable θ , Figures 21 and 22) do not significantly influence the coaptation profile. The results are more notable if we change the model formulation, especially for stiffer material ($\mu = 3000$ kPa). In all the considered cases, the shell formulation reduces the coaptation area and lengthens the coaptation zone along the free edge.

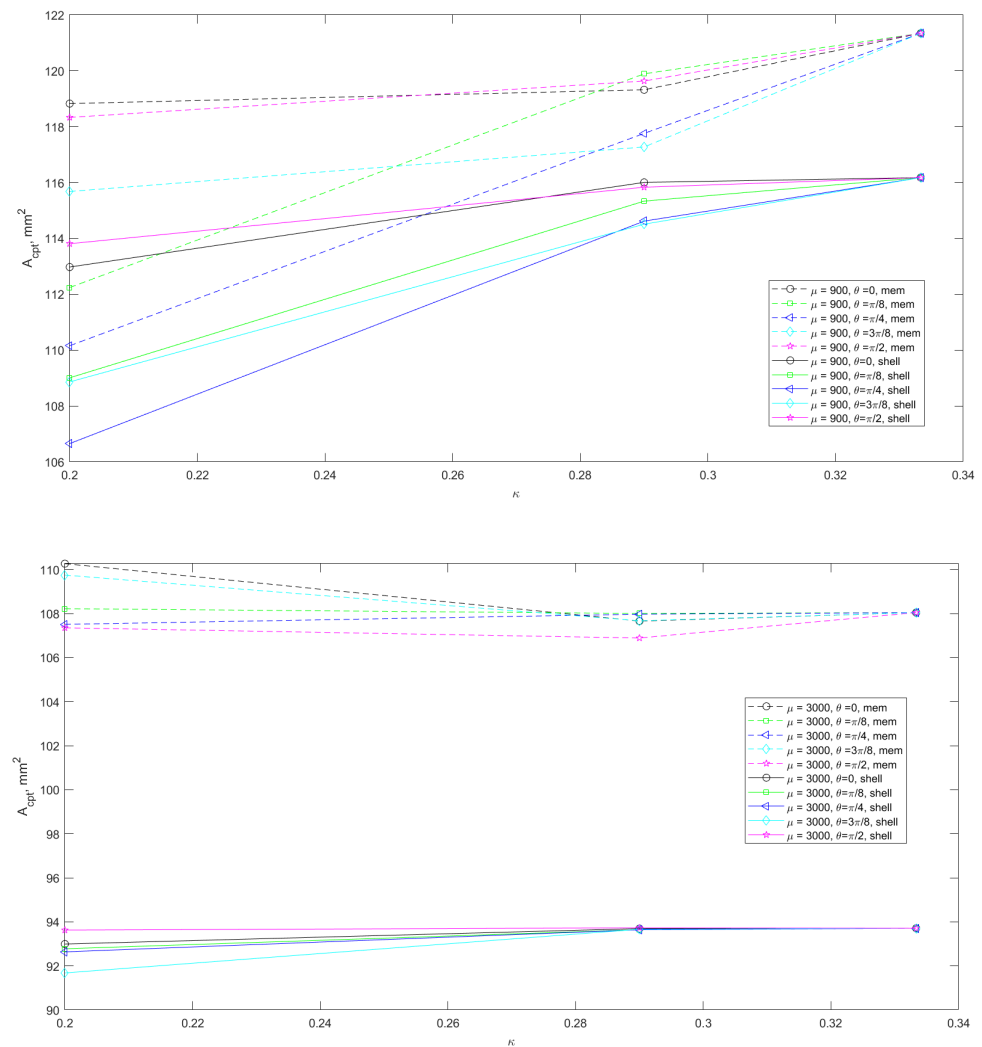


Figure 19. Coaptation area for different model parameters and model formulations.

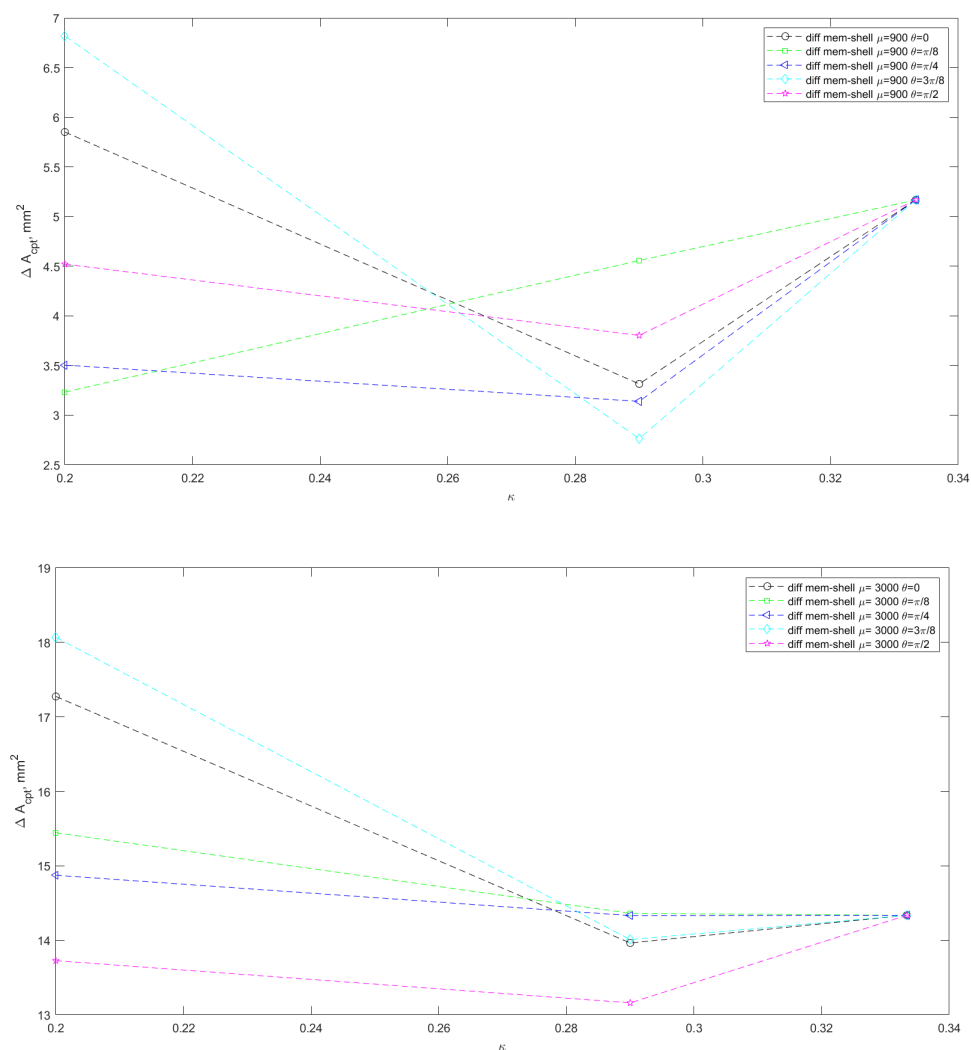


Figure 20. Difference of coaptation area (membrane-shell) for different model parameters.

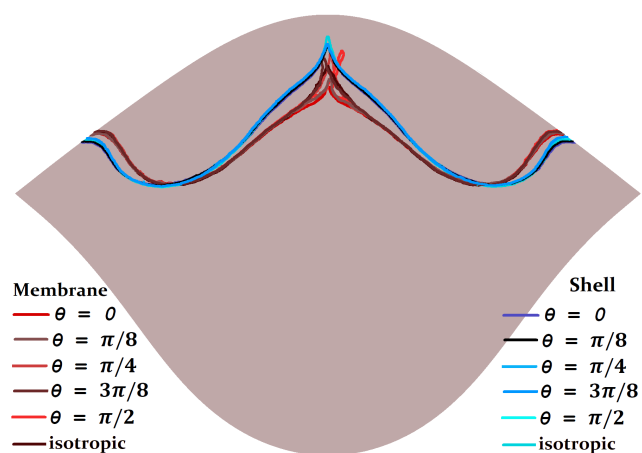


Figure 21. Coaptation profiles for $\mu = 900$ kPa, $\kappa = 0.29$, varied θ on the unfolded template. Profiles for membrane are almost the same except the central zone; profiles for shell are almost the same.

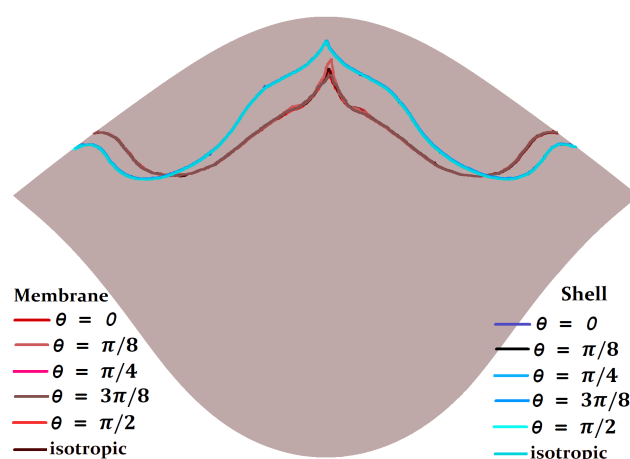


Figure 22. Coaptation profiles for $\mu = 3000$ kPa, $\kappa = 0.29$, varied θ on the unfolded template. Profiles for shell are superimposed on each other; profiles for membrane are almost the same.

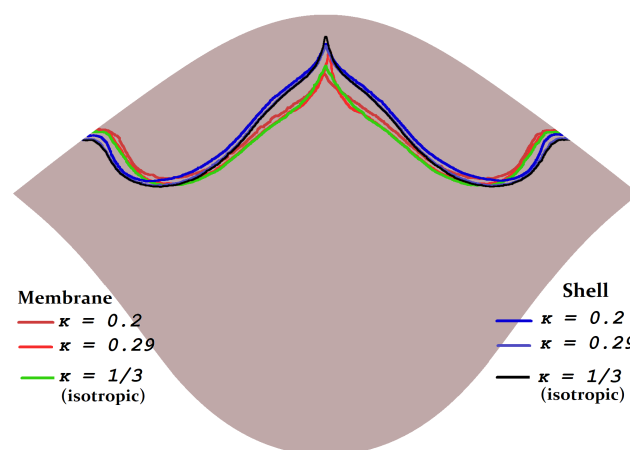


Figure 23. Coaptation profiles for $\mu = 900$ kPa, $\theta = \pi/4$, varied κ on the unfolded template.

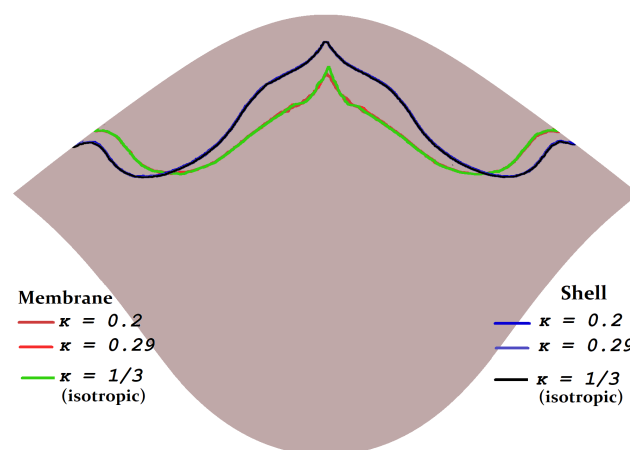


Figure 24. Coaptation profiles for $\mu = 3000$ kPa, $\theta = \pi/4$, varied κ on the unfolded template. Profiles for shell are superimposed on each other; profiles for membrane are almost the same.

4. Discussion

Both the competence of the reconstructed aortic valves and design leaflet optimization rely on the coaptation characteristics and diastolic valve configuration. These characteristics can be evaluated by the shell or membrane formulations. Some authors insist that “in-plane and flexural mechanical properties of the leaflets play an important role in the valvular function” [33] and thus, one should use the shell formulation. Others suggest that the

membrane is a feasible approximation: “we model the native leaflets and pericardium as membranes, assuming negligible flexural stiffness. This is supported by data showing bending stresses at least an order of magnitude smaller than in-plane stresses” [29]. For surgical neocuspidization planning, the membrane formulation is more preferable since it is easy to solve. However, it has to be validated by physical experiments. Moreover, the lack of solid knowledge on the mechanical properties of glutaraldehyde-treated human pericardium hampers the implementation of numerical models in clinical practice.

In our study, we want to explore how the reduced (shell/membrane) model and the leaflet material affects the coaptation zone and the diastolic configuration of the aortic valve. Additionally, we propose a method to compute the leaflet initial configuration, mimicking the real sutured neo-leaflet.

According to our results, the coaptation characteristics are sensitive to the model formulation, especially for stiff materials. The coaptation heights difference is larger (up to 1–2 mm) in the central zone of coaptation. The shell formulation provides usually a lesser coaptation zone than the membrane formulation. A discrepancy of 1–2 mm may be of the order of the central coaptation height. The future leaflet design optimization procedure should account for such a discrepancy. The area of the coaptation zone based on shell formulation is less than that based on membrane formulation: the difference for soft materials ($\mu = 900$ kPa) is up to 8% and for stiff materials ($\mu = 3000$ kPa) is up to 16%.

Anisotropy of the leaflet material does not affect significantly the coaptation characteristics; this result is similar to that of [28]. Anisotropy can impact the deformed leaflet configuration and produce smaller displacement. For some anisotropy directions, the displacement of the free edge and the belly region are significantly smaller compared to the isotropic case; this result agrees with similar findings for the pulmonary valve [37]. The material stiffness does influence the coaptation zone: it is smaller for stiffer material. Therefore, the study of mechanical properties of the treated human pericardium is highly demanded.

The limitation of our study is using contact planes instead of true leaflets contact, which reduces the computational complexity. Due to the symmetry, it is believed that the results would not change if one considers coaptation of all three leaflets. Validation of our mathematical models by physical experiments is to be performed. This is related to our future work.

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