

1       **Can we obtain *in vivo* transmural mean hoop stress of the aortic**  
2       **wall without knowing patient-specific material properties and**  
3       **residual deformations?**

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## 32 **Abstract**

33 It is well known that residual deformations/stresses alter the mechanical behavior of arteries, e.g.  
34 the pressure-diameter curves. In an effort to enable personalized analysis of the aortic wall stress,  
35 approaches have been developed to incorporate experimentally-derived residual deformations into  
36 *in vivo* loaded geometries in finite element simulations using thick-walled models. Solid elements  
37 are typically used to account for “bending-like” residual deformations. Yet, the difficulty in  
38 obtaining patient-specific residual deformations and material properties has become one of the  
39 biggest challenges of these thick-walled models. In thin-walled models, fortunately, static  
40 determinacy offers an appealing prospect that allows for the calculation of the thin-walled  
41 membrane stress without patient-specific material properties. The membrane stress can be  
42 computed using forward analysis by enforcing an extremely stiff material property as penalty  
43 treatment, which is referred to as the forward penalty approach. However, thin-walled membrane  
44 elements, which have zero bending stiffness, are incompatible with the residual deformations, and  
45 therefore, it is often stated as a limitation of thin-walled models. In this paper, by comparing the  
46 predicted stresses from thin-walled models and thick-walled models, we demonstrate that the  
47 transmural mean hoop stress is the same for the two models and can be readily obtained from *in*  
48 *vivo* clinical images without knowing the patient-specific material properties and residual  
49 deformations. Computation of patient-specific mean hoop stress can be greatly simplified by using  
50 membrane model and the forward penalty approach, which may be clinically valuable.

51 **Keywords:** residual stress; transmural mean hoop stress; membrane stress; forward penalty  
52 approach.

## 53 **1 Introduction**

54 Residual deformations/stresses first discovered in the 1980s (Chuong and Fung 1986;  
55 Vaishnav and Vossoughi 1983) have been shown to significantly affect the physiological wall  
56 stress distributions (Delfino et al. 1997; Fung 1991; Holzapfel et al. 2000; Humphrey 2002;  
57 Matsumoto and Hayashi 1996). To incorporate residual deformations in arteries, traditional  
58 forward analysis uses a thick-walled model starting from the stress-free reference configuration.  
59 Then deformation relations, constitutive laws and equilibrium equations are utilized to solve the  
60 boundary value problem. However, when applying this conventional approach to obtain patient-  
61 specific stress fields from the *in vivo* loaded geometries in clinical images, one has to first  
62 determine the unknown material parameters and residual deformations, which are required in the  
63 thick-walled finite element (FE) models. Some studies have suggested the use of experimentally-  
64 determined material and residual deformation parameters (Alastrué et al. 2010; Pierce et al. 2015).  
65 However, using residual deformations and material properties that are not patient-specific is a clear  
66 limitation.

67 Fortunately, for a specific type of biological membrane structures such as the aorta, the  
68 wall stress is nearly insensitive to the variation of material properties. This property is called static  
69 determinacy, i.e. the external force (pressure) along the geometry can be used to directly compute  
70 the internal tension/stress. This is because the vessel wall can be seen as locally in a plane stress  
71 state (Miller and Lu 2013), the solution of the equilibrium is weakly sensitive to the material  
72 properties. The aorta is shown to be approximately statically determinate (Joldes et al. 2016; Liu  
73 et al. 2017). Thus, its stress distribution can be directly obtained using membrane elements by a  
74 forward penalty method (Joldes et al. 2016; Lu and Luo 2016) which enforces an extremely stiff  
75 material property as penalty treatment. The computation of the thin-walled stress can be greatly

76 simplified by this forward approach. However, due to the assumption of no bending stiffness in  
77 the membrane elements, the self-equilibrium residual deformations are inadmissible to the thin-  
78 walled models, which is often stated as a limitation of such models.

79 In this paper, by comparing the predicted stresses from thin-walled models with thick-  
80 walled models considering residual deformations, we demonstrate that the transmural mean hoop  
81 stress (i.e., averaged stress through the thickness) fields are the same for the two models. Thus, the  
82 transmural mean hoop stress can be readily obtained from *in vivo* clinical images using the forward  
83 penalty approach without knowing the patient-specific material properties and residual  
84 deformations. The remaining sections are organized as follows. In Section 2, the theoretical  
85 arguments are described and the validity is shown by analytical examples. Thin-walled and thick-  
86 walled FE models with a patient-specific geometry are demonstrated in Section 3. In Section 4,  
87 the discussion and conclusions are presented.

## 88 **2 Theoretical and Analytical Arguments**

89 One prominent example of static determinacy is the use of Laplace law to compute the wall  
90 hoop stress by assuming a perfect cylindrical shape of the aorta.

$$91 \quad \sigma_{\theta\theta} = \frac{Pa}{t} \quad (1)$$

92 where  $\sigma_{\theta\theta}$  is the hoop stress in the thin-walled tube,  $P$  is the pressure,  $a$  is the inner radius, and  $t$   
93 is the *in vivo* wall thickness. The material properties are not involved in this equation, and stress  
94 is directly calculated using the static force equilibrium. Opposite to the middle radius value used  
95 in (Horný et al. 2014), we emphasize that inner radius should be used as the blood pressure is  
96 applied to the inner surface of the aorta.

97 It is well known that residual stresses alter the mechanical response of arteries, e.g. the  
98 pressure-diameter curves (Holzapfel et al. 2000). Nonetheless, from the static determinacy  
99 prospective, for the *in vivo* loaded configuration, the equilibrium between the resultant force and  
100 the external pressure load should always hold, and thus, the hoop stress resultant (tension) should  
101 be insensitive to the material parameters and residual deformations. This implies that no matter  
102 how the aorta is internally balanced or residually stressed, the wall tension can always be computed  
103 only using the static equilibrium. Therefore, when the wall thickness is given, the simple thin-  
104 walled model would be sufficient in determining the transmural mean hoop stress.

## 105 **2.1 The Opening Angle Method**

106 In this subsection, we use an analytical example to demonstrate that the mean hoop stress is  
107 insensitive to the change of opening angles. We assume that the residual stress can be described  
108 by the opening angle and that the aorta can be modelled as a perfect tube.

109 Starting from the cut-open, stress-free configuration, summarizing from (Holzapfel et al. 2000)  
110 and (Pierce et al. 2015), the total deformation gradient tensor of the tube taking into account the  
111 residual stress,  $\mathbf{F}_{total}$ , can be obtained as

$$112 \quad \mathbf{F}_{total}(r) = \frac{rk}{\left[A^2 + k\frac{l}{L}(r^2 - a^2)\right]^{\frac{1}{2}}} \mathbf{e}_\theta \otimes \mathbf{E}_\theta + \frac{l}{L} \mathbf{e}_z \otimes \mathbf{E}_Z + \frac{L}{rkl} \left[A^2 + k\frac{l}{L}(r^2 - a^2)\right]^{\frac{1}{2}} \mathbf{e}_r \otimes \mathbf{E}_R \quad (2)$$

113 where  $r \in [a, b]$ ,  $a$  and  $b$  are the inner and outer radii of the *in vivo* deformed geometry.  $k$ ,  
114 defined as  $k = \frac{2\pi}{2\pi - \alpha}$ , is used to describe the opening angle  $\alpha$ .  $A$  and  $B$  are the inner and outer radii  
115 of the stress-free geometry.  $L$  and  $l$  are the axial length of the aorta segment in the stress-free and  
116 deformed geometry, respectively.  $\mathbf{E}_\theta$ ,  $\mathbf{E}_Z$  and  $\mathbf{E}_R$  and  $\mathbf{e}_\theta$ ,  $\mathbf{e}_z$  and  $\mathbf{e}_r$  are the unit basis vectors for

117 the stress-free and deformed geometry respectively. To make the solution simple, the constitutive  
118 relation of the aorta tissue is modelled using the isotropic Neo-Hookean model. The strain energy  
119  $\Psi$  is

$$120 \quad \Psi = \frac{1}{2}\mu(I_1 - 3) \quad (3)$$

121 where  $\mu$  is the shear modulus and  $I_1$  is the first invariant. To solve for the *in vivo* stress when  
122 systolic blood pressure ( $P = 104\text{mmHg}$ ) (Martin et al. 2015) is present, we utilize the stress  
123 equilibrium equation, which can be expressed in the radial equation

$$124 \quad \frac{d\sigma_{rr}}{dr} = \frac{1}{r}(\sigma_{rr} - \sigma_{\theta\theta}) \quad (4)$$

125 where  $\sigma_{\theta\theta}$  and  $\sigma_{rr}$  are the stresses in the circumferential and radial direction respectively. Eqn. (4)  
126 can be reduced to  $\frac{d\sigma_{rr}}{dr} = \frac{\mu}{r}(\lambda_\theta^2 - \lambda_r^2)$  (Holzapfel and Ogden 2010), with  $\lambda_\theta$  and  $\lambda_r$  referring to the  
127 stretches in the circumferential and radial directions, respectively. By solving the equilibrium Eqn.  
128 (4), together with the traction continuity condition  $\sigma_{rr}(a) = -P$ , we are able to obtain the radial  
129 stress (Holzapfel and Ogden 2010)

$$130 \quad \sigma_{rr}(r) = -P + \mu \left[ \frac{k}{\lambda_z} \log\left(\frac{\lambda_r \lambda_z r k}{A}\right) - \frac{1}{k\lambda_z} \log\left(\frac{r}{a}\right) + \frac{1}{2} \left( \lambda_r^2 - \frac{1}{k\lambda_z} \right) \left( \frac{a^2 - r^2}{a^2} \right) \right] \quad (5)$$

131 where  $\lambda_z$  is the stretch in the axial direction. The hoop stress is then calculated using

$$132 \quad \sigma_{\theta\theta}(r) = \sigma_{rr}(r) + \mu(\lambda_\theta^2 - \lambda_r^2) \quad (6)$$

133 The geometry of the aorta in clinical images is always in the *in vivo* deformed state, from which  
134 the opening angle is not measurable. To this end, we fixed the inner and outer radii of the *in vivo*  
135 deformed geometry,  $a$  and  $b$ , for all scenarios and vary the opening angle from 0 to 330 degree.

136 For a certain opening angle  $\alpha$ , the inner and outer radii  $A$  and  $B$  of the cut-open sectors are

137 solved using the boundary condition  $\sigma_{rr}(b) = 0$  and the assumption of incompressibility  $b^2 =$   
138  $a^2 + \frac{1}{k\lambda_z}(B^2 - A^2)$ . Related parameters are listed in Table 1 and values of  $A$  and  $B$  are shown in  
139 Table 2. The transmural mean hoop stress is defined as

$$140 \quad \bar{\sigma}_{\theta\theta} = \frac{1}{b-a} \int_a^b \sigma_{\theta\theta} dr \quad (7)$$

141 The results are shown in Figure 1 (left). The mean hoop stress computed from Eqn. (7) is  
142 exactly the same as the thin-walled hoop stress calculated using Eqn. (1). Unsurprisingly, if we  
143 rewrite Eqn. (4) as  $\sigma_{\theta\theta} = \frac{d}{dr}(r\sigma_{rr})$  and therefore  $\bar{\sigma}_{\theta\theta} = \frac{1}{b-a} \int_a^b d(r\sigma_{rr}) = \frac{b\sigma_{rr}(b) - a\sigma_{rr}(a)}{t} = \frac{Pa}{t}$ ,  
144 which is exactly the same formula as the Laplace law. In addition, as shown in Figure 1 (right),  
145 the adoption of anisotropic constitutive model (the GOH model (Gasser et al. 2006), described in  
146 Section 3.2.1, parameters shown in Table 3) would not affect the static determinacy. The inner  
147 hoop stress tends to be reduced while the outer hoop stress is increased when gradually increasing  
148 the opening angle. Here, small opening angles may be unusual to observe in experiment (Sokolis  
149 2015), they are presented here for illustrative purpose.

## 150 **2.2 The Layer-Specific Three-Dimensional Residual Stress Model**

151 As a step forward, (Holzapfel and Ogden 2010) proposed a layer-specific three-  
152 dimensional residual stress model, in which the residual deformations (stretching and bending) of  
153 the three layers (intima, media and adventitia) from (Holzapfel et al. 2007) were encompassed and  
154 the residual stresses were calculated using the isotropic Neo-Hookean model. In this section, we  
155 first replicate the stress distribution in (Holzapfel and Ogden 2010) by using the original  
156 parameters of geometry, material and residual deformations. Next, physiological pressure is

157 applied to the residually-stressed aorta. The result indicates that the transmural mean hoop stress  
 158 is independent of residual deformations.

159 The deformation gradient tensors for intima (I), media (M) and adventitia (A) (Pierce et al.  
 160 2015) are

$$161 \mathbf{F}_{RS}^{(I)}(r^{(I)}) = \frac{r^{(I)k^{(I)}}}{\left[A^{(I)2} + k^{(I)} \frac{l}{L^{(I)}} (r^{(I)2} - a^{(I)2})\right]^{\frac{1}{2}}} \mathbf{e}_\theta \otimes \mathbf{E}_\theta + \frac{l}{L^{(I)}} \mathbf{e}_z \otimes \mathbf{E}_z + \frac{L^{(I)}}{r^{(I)k^{(I)}l} \left[A^{(I)2} + k^{(I)} \frac{l}{L^{(I)}} (r^{(I)2} - \right. \\ 162 \left. a^{(I)2})\right]^{\frac{1}{2}}} \mathbf{e}_r \otimes \mathbf{E}_R$$

$$163 \mathbf{F}_{RS}^{(M)}(r^{(M)}) = \frac{r^{(M)\beta}}{L^{(M)}} \mathbf{e}_\theta \otimes \mathbf{E}_z + \frac{l^{(M)k^{(M)}}}{\pi \left[A^{(M)2} + \frac{\beta l^{(M)k^{(M)}}}{\pi L^{(M)}} (b^{(M)2} - r^{(M)2})\right]^{\frac{1}{2}}} \mathbf{e}_z \otimes \mathbf{E}_\theta + \frac{\pi L^{(M)}}{r^{(M)\beta l^{(M)k^{(M)}}} \left[A^{(M)2} + \right. \\ 164 \left. \frac{\beta l^{(M)k^{(M)}}}{\pi L^{(M)}} (b^{(M)2} - r^{(M)2})\right]^{\frac{1}{2}}} \mathbf{e}_r \otimes \mathbf{E}_R$$

$$165 \mathbf{F}_{RS}^{(A)}(r^{(A)}) = \frac{\pi r^{(A)}}{L_2^{(A)}} \mathbf{e}_\theta \otimes \mathbf{E}_{X_2} + \frac{l}{L_3^{(A)}} \mathbf{e}_z \otimes \mathbf{E}_{X_3} + \frac{L_2^{(A)} L_3^{(A)}}{\pi r^{(A)} l} \mathbf{e}_r \otimes \mathbf{E}_{X_1} \quad (8)$$

166 The definitions and values of the parameters are referred to (Holzapfel and Ogden 2010). Values  
 167 of the related parameters are listed in Table 4.

168 Similar to the procedures for the opening angle method, the hoop stress can be computed  
 169 using the equilibrium equation and the boundary conditions. Interested readers are referred to  
 170 (Holzapfel and Ogden 2010) for details. A diastolic pressure ( $P = 80mmHg$ ) is applied to the  
 171 inner surface of the aorta, and we assume no axial tension caused by *in vivo* loading conditions.  
 172 The residual axial stretches have been incorporated in the deformation gradient tensors of each  
 173 layer. The transmural mean hoop stress for the three layer composite is defined as

$$174 \bar{\sigma}_{\theta\theta} = \frac{1}{b^{(A)} - a^{(I)}} \sum_{i=I,M,A} \int_{a^{(i)}}^{b^{(i)}} \sigma_{\theta\theta}^{(i)} dr \quad (9)$$



175 As depicted in Figure 2, the mean hoop stress is identical to the thin-walled hoop stress.

### 176 **3 Finite Element Analyses Incorporating Residual Deformations**

177 In this section, irregularity of patient-specific geometries are taken into account using FE  
178 analyses. The validity of the conclusion in Section 2 is examined by a real patient geometry. The  
179 forward penalty approach (Section 3.1) is used to estimate the thin-walled membrane stress. For  
180 the thick-walled FE models, the generalized pre-stressing algorithm (GPA) (Pierce et al. 2015;  
181 Weisbecker et al. 2014) is implemented in ABAQUS (Section 3.2) to predict the *in vivo* stress  
182 distribution with both the residual deformations and the pre-stresses incorporated.

183 A CT-derived geometry from the ascending thoracic aortic aneurysm (ATAA) patient  
184 (Martin et al. 2015) were used. The inner surface of the aortic wall was divided into 4,950 M3D4  
185 membrane elements in ABAQUS, using the automatic algorithm (Liang et al. 2017) previously  
186 developed by our group. Mesh sensitivity analysis was performed in our previous work (Martin et  
187 al. 2015). Due to partial volume effect, the wall thickness is difficult to infer from CT images,  
188 therefore a constant deformed thickness of 1.5 mm was assumed based on (Liang et al. 2017).  
189 Sensitivity analyses with respect to the wall thickness were carried out in Section 3.2.2. Next, the  
190 membrane mesh was extruded outwardly to create two solid meshes (C3D8 elements) with 8 and  
191 9 layers in Section 3.2.2 and Section 3.2.3, respectively.

#### 192 **3.1 A Thin-walled Model using the Forward Penalty Approach**

193 The prediction of the *in vivo* stress of the aortic wall has been relied on the recovery of the unloaded  
194 state and the incorporation of residual deformations, which requires the use of iterative techniques  
195 (Alastrué et al. 2010). A simple and effective forward penalty approach (Joldes et al. 2016) (Lu

196 and Luo 2016) has been recently proposed to predict the *in vivo* membrane stress without knowing  
197 the material properties. In statically determinant structures, the stress is independent of the material  
198 properties, it would be legitimate to assume an extremely stiff property, so that the  
199 deformation/change of shape from the unloaded configuration to the loaded configuration is  
200 infinitesimal/negligible. This allows us to use the *in vivo* configuration as the unloaded  
201 configuration because the deformation is infinitesimal. In the forward method, an artificially stiff  
202 material property (i.e.  $\mu = 10^7 Pa$ , Neo-Hookean model) is assigned to the aortic wall, realizing a  
203 penalty treatment to enforce a nearly rigid condition (Lu and Luo 2016). When the *in vivo* pressure  
204 is applied to the *in vivo*, image-derived geometry, the deformation would be infinitesimal due to  
205 the high stiffness of the material. The correct *in vivo* membrane stress field is readily obtained in  
206 this forward analysis due to the fact that the aortic wall is approximately statically determinate.  
207 This approach was shown as effective as iterative approach (Lu and Luo 2016).

208         Similar to the reason for the use of the inner radius in the Laplace equation (Eqn. (1)), we  
209 emphasize that the inner surface of the aortic wall should be used in the thin-walled model when  
210 applying the forward approach.

## 211 **3.2 Thick-walled Models Incorporating Residual Deformations**

### 212 **3.2.1 Method to incorporate Residual Deformations to Thick-walled** 213 **Models**

214         The aortic tissue is described by the Gasser-Ogden-Holzapfel (GOH) model (Gasser et al.  
215 2006)

$$216 \quad \Psi = C_{10}(\bar{I}_1 - 3) + \frac{k_1}{2k_2} \sum_{i=1}^2 \left[ \exp \left\{ k_2 \left[ \kappa \bar{I}_1 + (1 - 3\kappa) \bar{I}_{4(6)} - 1 \right]^2 \right\} - 1 \right] + \frac{1}{D} \left[ \frac{J^2 - 1}{2} - \ln J \right] \quad (10)$$

217 where  $C_{10}$ ,  $k_1$ ,  $k_2$  and  $\kappa$  are material parameters,  $\theta$  defines the fiber directions, please refer to  
218 (Abaqus 2014; Gasser et al. 2006) for detailed definitions. The parameter  $D$  enforces the nearly  
219 incompressibility and is fixed to be  $1 \times 10^{-5}$ .

220 The GPA (Pierce et al. 2015; Weisbecker et al. 2014) is utilized to incorporate the residual  
221 deformation. The total deformation gradient  $\mathbf{F}_t$  is stored as a history variable for each integration  
222 point.  $\mathbf{F}_t$  is updated based on the incremental deformation gradient  $\Delta\mathbf{F}$  resulting from the  
223 prescribed load and boundary conditions.

$$224 \quad \mathbf{F}_{t+1} = \Delta\mathbf{F}\mathbf{F}_t \quad (11)$$

225 The incremental deformation gradient of the residual stress  $\Delta\mathbf{F}_{RS}$  is first iteratively applied to the  
226 image-derived geometry and stored in  $\mathbf{F}_t$ . Next, the incremental deformation gradient of the pre-  
227 stress  $\Delta\mathbf{F}_{PS}$  resulting from the *in vivo* blood pressure is incrementally applied and stored in  $\mathbf{F}_t$ .  
228 Thus, deformation gradient tensors associated with the residual stress  $\mathbf{F}_{RS}$  and the pre-stress  $\mathbf{F}_{PS}$   
229 are accounted sequentially. The GPA is implemented in the ABAQUS user subroutine UMAT.  
230 The implementation was validated by comparing the analytical and FE results as in (Pierce et al.  
231 2015).

### 232 **3.2.2 Thick-walled Models with Various Opening Angles**

233 The thick-walled solid elements were utilized in this section to encompass the opening  
234 angle. Various values of the opening angle were incorporated through the GPA. Small opening  
235 angles may be unusual to observe in experiments, they are shown here for illustration purposes.  
236 The aorta was modelled as a single layer wall. This assumption may be relevant to abdominal  
237 aneurysmal tissue since collagen structure becomes nearly homogenous across the entire wall

238 (Gasser et al. 2012). For ascending aortic aneurysms, collagen organization may be different in  
239 different layers (Sassani et al. 2015). The GOH model (Eqn (10)) was used as the constitutive law,  
240 and the material parameters (shown in Table 3) were determined from fitting the biaxial data from  
241 (Martin et al. 2015) of the particular patient.

242 Mean absolute percentage error (MAPE) was used to compare the transmural mean hoop  
243 stress (Eqn.(7)) of the thin-walled and thick-walled models:

$$244 \quad MAPE = \frac{1}{N} \sum_{i=1}^N \left| \frac{\bar{\sigma}_{\theta\theta,i}^{(thin)} - \bar{\sigma}_{\theta\theta,i}^{(thick)}}{\bar{\sigma}_{\theta\theta,i}^{(thin)}} \right| \quad (12)$$

245 where  $\bar{\sigma}_{\theta\theta,i}^{(thin)}$  and  $\bar{\sigma}_{\theta\theta,i}^{(thick)}$  are the transmural mean hoop stress predicted by the thin-  
246 walled and thick-walled models respectively.  $i$  is an element index for the thin-walled model and  
247  $N$  is the number of elements.

248 To study the sensitivity of the MAPE of the transmural mean stress with respect to the  
249 thickness, three representative thickness values (1mm, 2mm and 3mm) were chosen with  $\alpha =$   
250  $120^\circ$ . The results are summarized in Table 5. Note that this opening angle value is chosen because  
251 the corresponding stress distribution is close to homogenized state in the FE simulation, and this  
252 value may not be consistent with the average value obtained from experiment (Sokolis 2015). We  
253 also notice that opening angle values are widely distributed according to (Sokolis 2015), 120  
254 degree can be considered as a feasible value.

255 In order to quantify the transmural variation, we define a signed transmural percentage  
256 error (STPE), corresponding to the  $i$ th thin-walled membrane element, as

$$257 \quad STPE(i) = sign[\sigma_{\theta\theta,i}^{(thick)}(a_i) - \sigma_{\theta\theta,i}^{(thick)}(b_i)] \frac{1}{b_i - a_i} \int_{a_i}^{b_i} \left| \frac{\sigma_{\theta\theta,i}^{(thick)}(r) - \bar{\sigma}_{\theta\theta,i}^{(thick)}}{\bar{\sigma}_{\theta\theta,i}^{(thick)}} \right| dr \quad (13)$$

258 where  $a_i$  and  $b_i$  represent the inner and outer radii respectively, and  $r$  is the radius. The sign is  
259 given based on the difference between the inner and outer wall hoop stress. If the inner wall stress  
260 is greater than the outer, the STPE is positive, otherwise the STPE is negative.

261 The results are shown in Figure 3, the transmural mean hoop stress fields are almost  
262 identical for various opening angles and the forward penalty approach. More detailed views of ring  
263 cuts at the same location are shown in Figure 4. With increased opening angle, the mean signed  
264 transmural percentage error (MSTPE) changes from positive to negative.

265 The probability density functions (PDFs) of the STPE are plotted in Figure 5. The PDFs  
266 are fitted using the Gaussian distribution. It can be observed that the PDF shifts leftward with the  
267 increase of the opening angle.

### 268 **3.2.3 A Thick-walled Model with Layer-Specific Three-Dimensional** 269 **Residual Deformation**

270 In this section, the deformation gradient tensors  $F_{RS}^{(i)}$  ( $i = I, M, A$ ) of Section 2.2 was  
271 incorporated in a FE simulation using the GPA. The ratio of intima, media and adventitia (18.53%,  
272 45.56%, 35.91%) and the layer-specific GOH parameters (shown in Table 6) were taken from the  
273 median experimental value for human thoracic aortas in (Weisbecker et al. 2012). Layer-specific  
274 material parameter data for ATAA is also available in (Sassani et al. 2015; Sokolis et al. 2012).  
275 The geometrical parameters determining the residual deformation of abdominal aorta from  
276 (Holzapfel and Ogden 2010), same as Section 2.2 (Table 4), were directly used for the ATAA  
277 patient. (Sokolis 2015) documented layer-specific residual stretch and opening angle data for  
278 ATAA. Unfortunately, it is not compatible with the current three-dimensional residual stress model

279 (Holzapfel and Ogden 2010). Specifically, (Holzapfel and Ogden 2010) considered different  
280 geometries of reference configurations for different layers and would need more complicated  
281 experimental setups.

282         Regardless of the discrepancy of the stress in the thickness direction (Figure 6, first row),  
283 the transmural mean stress field predicted by the forward penalty approach and the GPA are, again,  
284 almost identical, with a MAPE of 3.98% (Figure 6, second row). Since the details of transmural  
285 distribution of hoop stress is not clearly shown in the first row of Figure 6, we use Figure 7 to show  
286 hoop stress distributions in a ring predicted by method described in Section 3.1 (forward,  
287 membrane), Section 3.2.2 (opening angle  $\alpha = 180^\circ$ ) and Section 3.2.3 (layer-specific 3D residual  
288 deformation), respectively.

## 289 **4 Discussions and Conclusions**

290         One of the biggest obstacles in the field of biomechanical analysis of the aorta is the  
291 difficulty in obtaining both the patient-specific material properties and the patient-specific residual  
292 deformations from *in vivo* clinical images. This paper offers an appealing prospect that the mean  
293 hoop stress (or hoop wall tension) of the aortic wall can be computed without knowing the  
294 mechanical properties and the residual deformations of the aortic tissue. Computation of patient-  
295 specific mean hoop stress can be greatly simplified by using membrane model and the forward  
296 penalty approach, which may be clinically valuable. In some wall strength tests (Ferrara et al. 2016;  
297 Pham et al. 2013), the intact wall is tested without separation of each individual layer, which  
298 corresponds to the averaged wall strength across the wall thickness, consistent with the membrane  
299 assumption. The mean hoop stress may be used together with the experimentally-obtained strength

300 to calculate an approximation of rupture risk such as the rupture potential index (RPI) (Vande  
301 Geest et al. 2006).

302 Because of the difference in constituents and thus mechanical properties, the hoop stress  
303 distribution may not be uniform in multi-layer models. The iterative approaches such as the GPA,  
304 may yield detailed results with through-thickness and layer-specific stress distributions using  
305 multilayered thick-walled models. Therefore, it would be natural to combine layer-specific wall  
306 stress distribution with available layer-specific wall strength data (Sokolis et al. 2012) for a more  
307 detailed rupture/dissection analysis. Nonetheless, residual deformations are shown to be highly  
308 patient-specific and axial location-dependent (Sokolis 2015). Elastic properties also exhibit  
309 regional (Iliopoulos et al. 2009; Sassani et al. 2015) and intra-patient (Martin et al. 2015) variations.  
310 Thus, such complex patient- and layer-specific residual deformation and elastic property fields  
311 need to be noninvasively estimated for an accurate modeling prediction of clinical events (e.g.  
312 rupture). Currently, it is impossible to estimate the layer-specific and heterogeneous material and  
313 residual deformation parameters simultaneously from *in vivo* clinical images. We admit that hoop  
314 stress within each layer may be more useful than mean hoop stress for predicting some clinical  
315 adverse events such as aortic dissection. However, the mean hoop stress is clinically valuable too  
316 because it is patient-specific, which does not depend on material parameters and residual  
317 deformations.

318 The inclusion of residual deformation often reduces the hoop stress gradient, and thus tends  
319 to homogenize the hoop stress distribution in the *in vivo* deformed configuration (Chaudhry et al.  
320 1997; Chuong and Fung 1986; Fung 1991; Holzapfel et al. 2000; Humphrey 2002; Raghavan et al.  
321 2004). This makes the thin-walled hoop stress, or the mean hoop stress more physiologically  
322 relevant in the sense that it represents the ideal homogenized wall stress in single layer models.

323 Homogenized stress state is an assumption for some growth models, e.g., (Polzer et al. 2013), and  
324 the method proposed in (Schröder and Brinkhues 2014) is based on smoothing the stress gradient.  
325 In this study, the incorporation of opening angles also tends to homogenize the hoop stress  
326 distribution as shown in Figure 1. In Figure 3, the MSTPE is close to 0 when 120~180 degree  
327 opening angle is incorporated. However, this value seems to be lower than the average value  
328 obtained from experiment (Sokolis 2015). This might be due to the assumption of uniform material  
329 properties and uniform thickness in the computational model, which could impact the transmural  
330 stress distribution. We also notice that a wide range of opening angle is documented in (Sokolis  
331 2015), 120~180 degree opening angle can be considered feasible.

332 The transmural mean axial/longitudinal stress of the aorta may be statically determinant  
333 when the longitudinal force is known. The ascending aorta also has *in vivo* longitudinal  
334 deformations/stretching due to the heart movements during cardiac cycles. Such boundary condition  
335 is very complex and it can be difficult to model in a FE simulation. In the present study, a simplified  
336 boundary condition was used: the boundary nodes were only allowed to move in the radial  
337 directions. We have tried different boundary conditions such as prescribing the longitudinal forces,  
338 but encountered convergence problems in the FE simulations. The *in vivo* longitudinal boundary  
339 conditions would significantly impact the longitudinal stress field, which warrants further studies  
340 in the future.

341 In conclusion, due to static determinacy, the transmural mean hoop stress in the *in vivo*  
342 configuration of the aorta is independent of mechanical properties and residual deformations. The  
343 forward penalty method, which enforces a rigid condition as the penalty treatment, can greatly  
344 simplify the computation of the mean hoop stress for patient-specific geometries.



## 345 **5 Acknowledgements**

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## 348 **6 Conflict of Interest**

349 The authors declare that they have no conflict of interest.

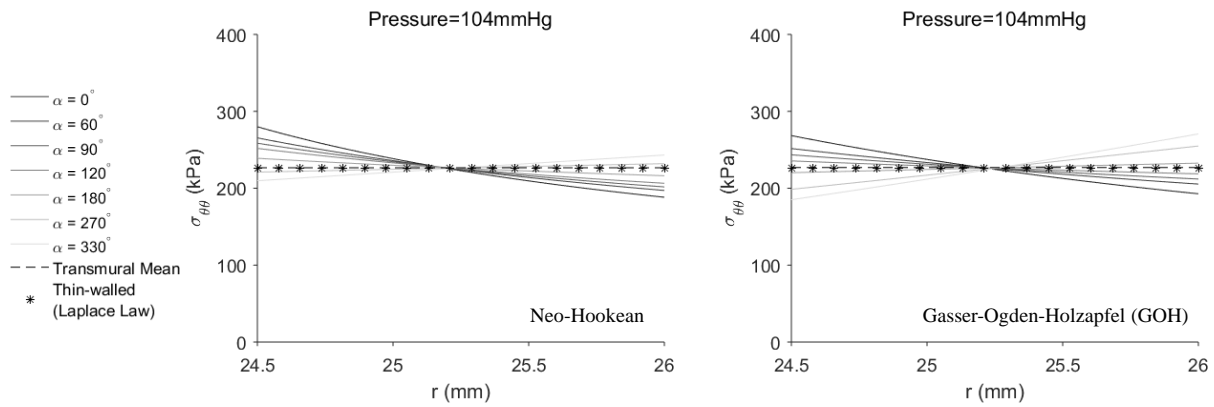
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454

455 Figure 1 the transmural mean, thin-walled and thick-walled hoop stresses across the wall thickness.

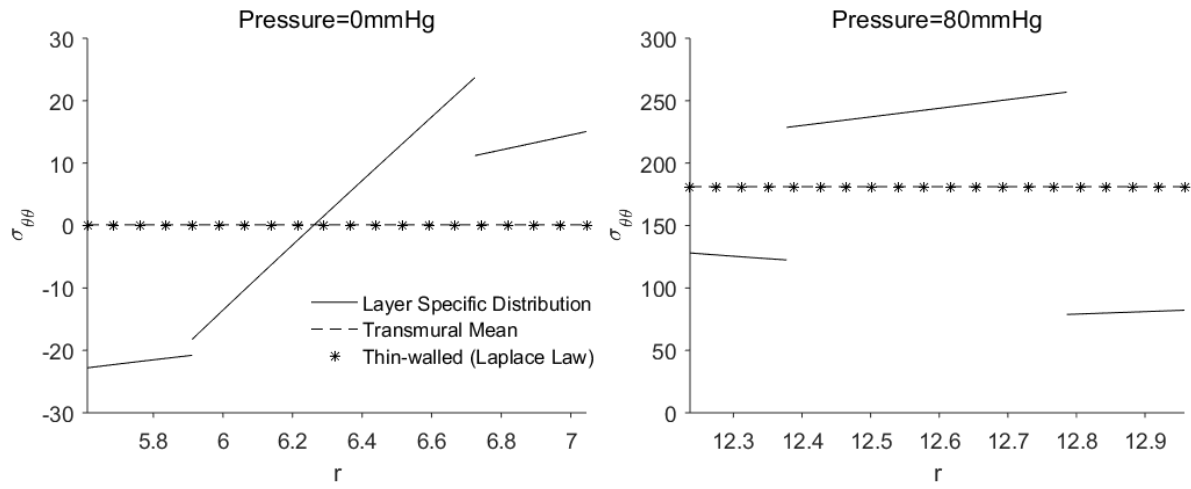
456 In the left figure, thick-walled hoop stresses were computed using Neo-Hookean model, while in

457 the right figure, GOH model was used. Transmural mean hoop stress remains the same for all

458 scenarios, thus only one line is plotted.

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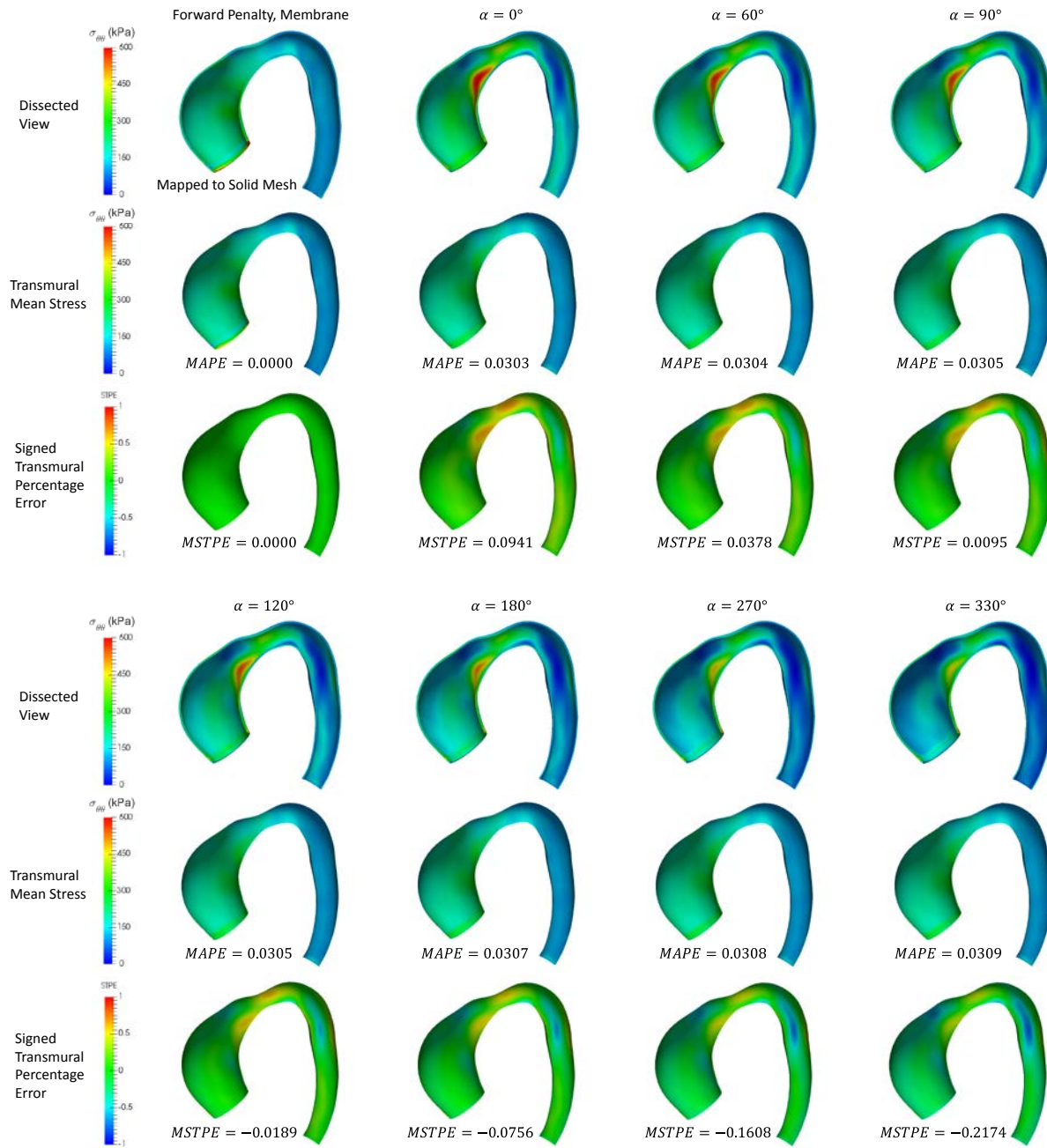


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462 Figure 2 the transmural mean, thin-walled and layer-specific hoop stress distributions in the three  
463 layer composite wall when 0 and 80 mmHg pressures are applied.

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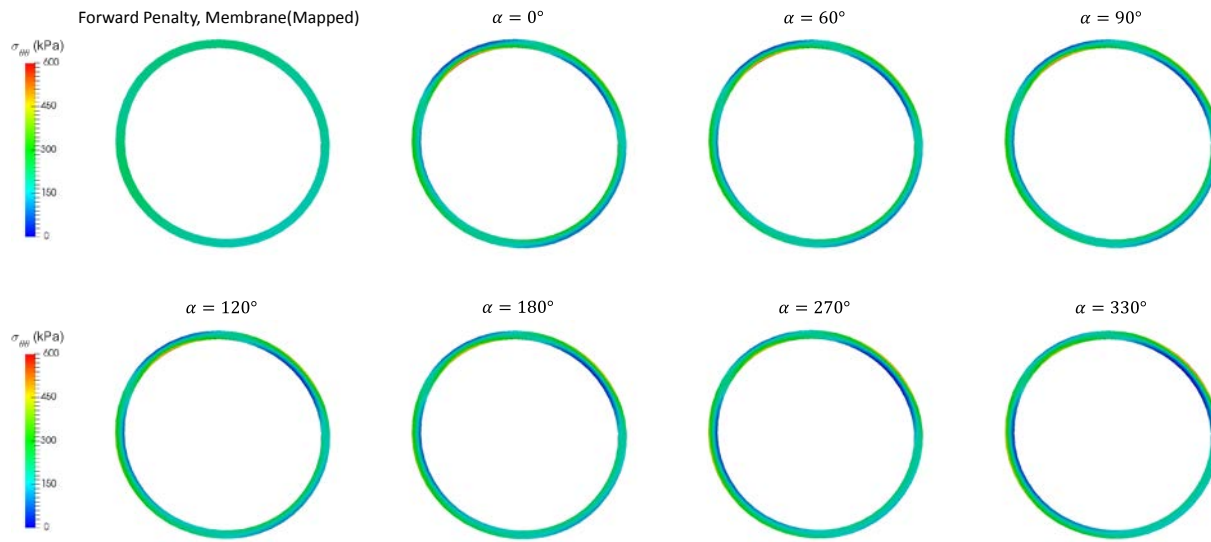
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467 Figure 3 predicted results using the forward penalty approach and the GPA approach with different  
468 opening angles: (1) the hoop stress distribution in the dissected view (row 1 and row 4), (2) the  
469 transmural mean hoop stress (row 2 and row 5), and (3) the signed transmural percentage error  
470 (row 3 and row 6).

471



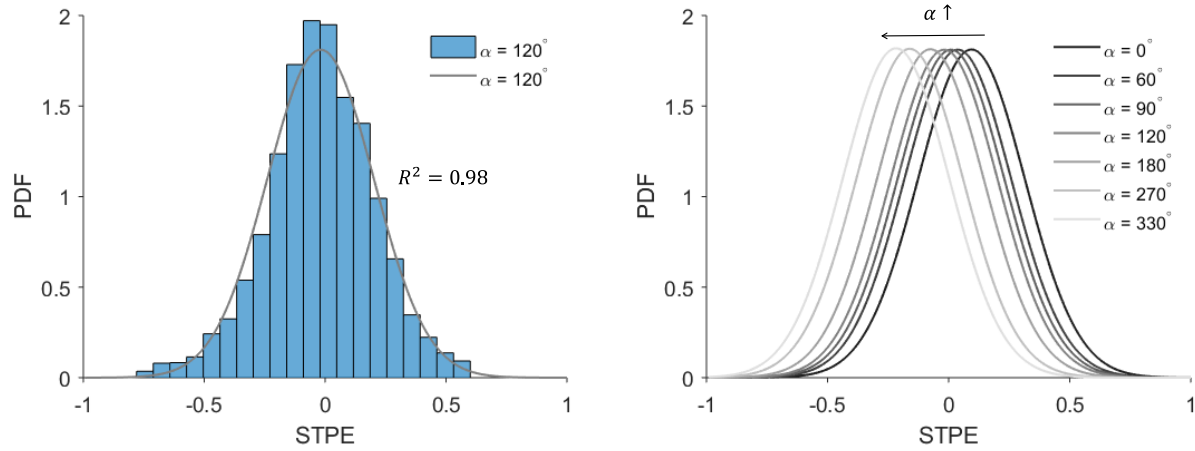
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473 Figure 4 hoop stress in aortic rings using the forward penalty approach and the iterative approach

474 (GPA) with different opening angles.

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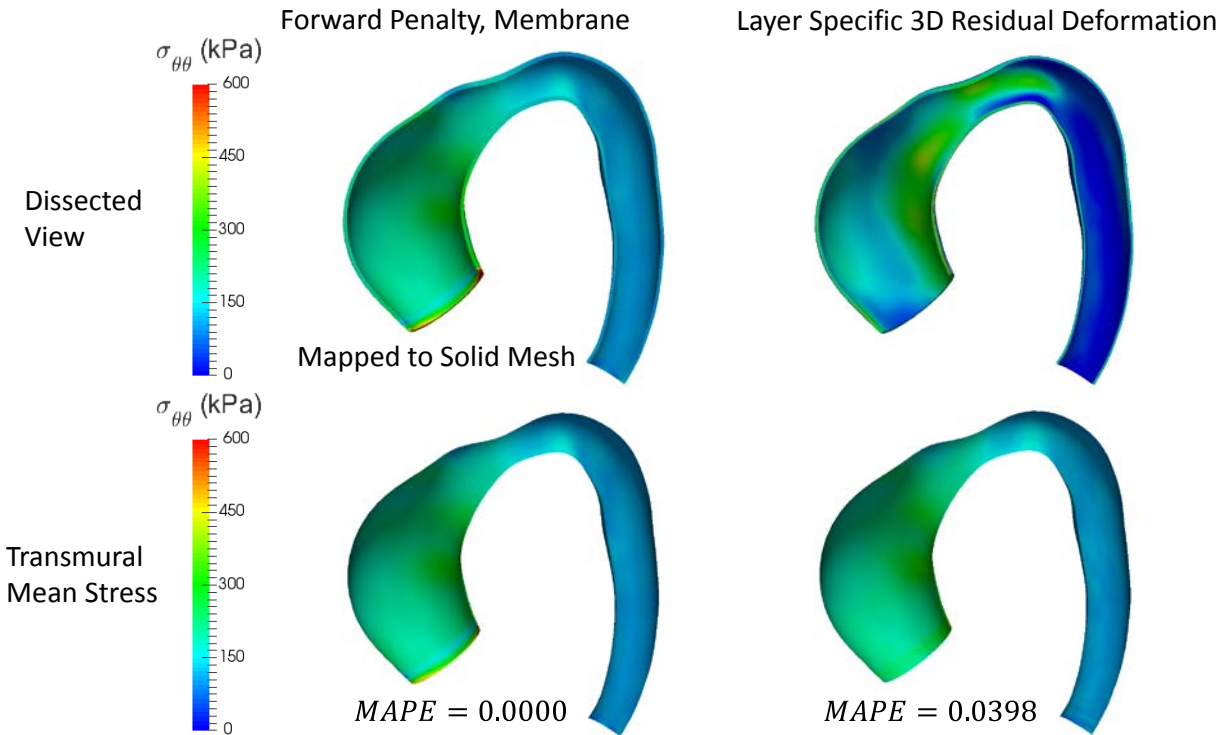
479 Figure 5 the probability density function (PDF) of the STPE is shown in the histogram and fitted

480 using the Gaussian distribution (left) and fitted PDFs correspond to different opening angles (right).

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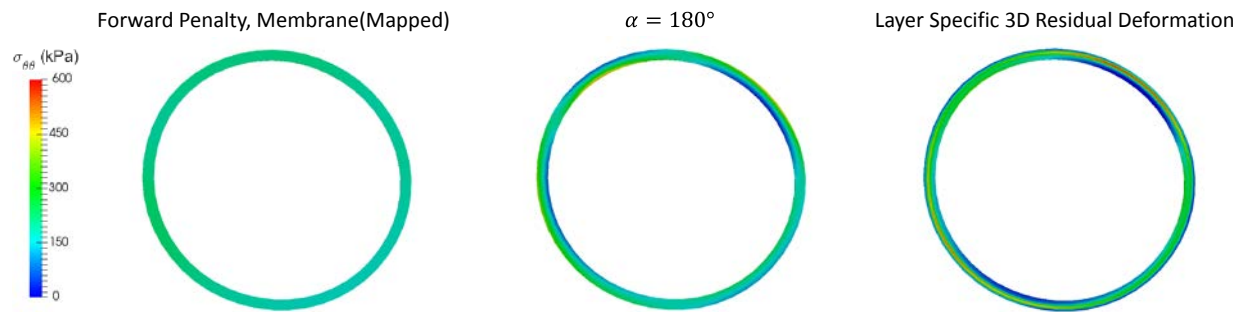


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483 Figure 6 predicted results using the forward penalty approach and the iterative approach (GPA)  
484 with layer-specific three-dimensional residual deformations: (1) the hoop stress distribution in the  
485 dissected view (row 1), (2) the transmural mean hoop stress (row 2).

486

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488

489 Figure 7 the hoop stress distribution in the aortic rings using the forward approach, the opening

490 angle method ( $\alpha = 180^\circ$ ) and the layer-specific 3D residual deformation.

491

492

inner radius $a$ (mm)	outer radius $b$ (mm)	residual axial stretch $l/L$	systolic pressure (mmHg)	shear modulus $\mu$ (kPa)
24.5 <sup>a</sup>	26 <sup>b</sup>	1.2 <sup>c</sup>	104 <sup>a</sup>	67.68 <sup>a</sup>

493 <sup>a</sup> from (Martin et al. 2015),  $a$  and systolic pressure are from clinical recorded data,  $\mu$  was fitted  
494 using biaxial experiment of patient “BAV17” with coefficient of determination of 0.8656; <sup>b</sup> based  
495 on mean value of deformed wall thickness in (Liang et al. 2017); <sup>c</sup> approximated from (Guo and  
496 Kassab 2003) which refers to the residual axial stretch. We assume there is no axial tension caused  
497 by *in vivo* loading conditions

498 Table 1 the parameters used in the opening angle method.

499

Neo-Hookean Model							
$\alpha(^{\circ})$	0	60	90	120	180	270	330
$A(mm)$	11.55	14.20	15.96	18.16	24.77	51.23	157.10
$B(mm)$	14.98	17.62	19.39	21.59	28.20	54.67	160.54
Gasser-Ogden-Holzapfel (GOH) Model							
$\alpha(^{\circ})$	0	60	90	120	180	270	330
$A(mm)$	18.25	22.12	24.70	27.93	37.63	76.43	231.66
$B(mm)$	20.59	24.46	27.04	30.26	39.97	78.77	234.00

500 Table 2 the inner and outer radii  $A$  and  $B$  of the stress-free configurations corresponding to  
501 various opening angles  $\alpha$ .

502

$C_{10}(kPa)$	$k_1(kPa)$	$k_2$	$\kappa$	$\theta(^{\circ})$
27.91	512.56	0.00	0.31	90.00

503 Table 3 GOH material parameters of the patient “BAV17” extracted from (Martin et al. 2015).

504 Coefficient of determination of the curve fitting is 0.9551.

505

Intima	Media	Adventitia
$A^{(I)} = 7.50mm$	$A^{(M)} = 8.41mm$	$L_1^{(A)} = 0.21mm$
$B^{(I)} = 7.76mm$	$B^{(M)} = 8.99mm$	$L_2^{(A)} = 18.35mm$
$L^{(I)} = 2.58mm$	$L^{(M)} = 2.52mm$	$L_3^{(A)} = 2.29mm$
$k^{(I)} = 1.19$	$k^{(M)} = 2.79$	$b^{(A)} = 7.05mm$
$a^{(I)} = 5.61mm$	$\mu^{(M)} = 31.4kPa$	$\mu^{(A)} = 17.3kPa$
$\mu^{(I)} = 39.8kPa$		

506 Table 4 material and residual deformation parameters from (Holzapfel and Ogden 2010;  
507 Holzapfel et al. 2007). In addition,  $l = 2.48mm$ ,  $b^{(I)} = a^{(M)}$  and  $b^{(M)} = a^{(A)}$  can be calculated  
508 according to (Holzapfel and Ogden 2010).

509

Wall thickness (mm)	1.0	2.0	3.0
MAPE	0.0191	0.0355	0.0458

510 Table 5 sensitivity of MAPE w.r.t. the thickness.

511

512

	$C_{10}$ (kPa)	$k_1$ (kPa)	$k_2$	$\kappa$	$\theta$ (°)
Intima	17	4340	13.32	0.20	46.5
Media	14	140	11.90	0.21	38.4
Adventitia	10	390	6.79	0.23	52.3

513 Table 6 layer-specific GOH material parameters from (Weisbecker et al. 2012).

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