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### Development and evaluation of a new procedure for subject-specific tensioning of finite element knee ligaments

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## Research Article

**Development and evaluation of a new procedure for subject-specific tensioning of  
finite element knee ligaments****AUTHORS**

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1  
2  
3 26 **Abstract**  
4

5 27 Subject-specific tensioning of ligaments is essential for the stability of the knee joint and  
6  
7 28 represents a challenging aspect in the development of finite element models. We aimed to  
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9  
10 29 introduce and evaluate a new procedure for the quantification of ligament prestrains from  
11  
12 30 biplanar X-ray and CT data. Subject-specific model evaluation was performed by comparing  
13  
14 31 predicted femorotibial kinematics with the *in vitro* response of six cadaveric specimens. The  
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16 32 differences obtained using personalized models were comparable to those reported in similar  
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18 33 studies in the literature. This study is the first step towards the use of simplified, personalized  
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20 34 knee FE models in clinical context such as ligament balancing.  
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30 37 **Keywords**

31 38 Finite Element Analysis, Ligament Prestrain, Subject-Specific Knee Model, Joint Kinematics,  
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## 1. Introduction

The knee joint is highly susceptible to frequent injury of ligaments. If it remains untreated, has the probability of limiting joint stability, and can further lead to progression of joint arthritis (Fleming et al. 2005). In such scenario, early stage clinical intervention e.g., ligament repair or replacement is often recommended. For such therapeutic interventions and to properly plan surgical procedures, accurate knowledge of the biomechanical behavior of knee ligaments is fundamental.

Several experiments dealing with main knee ligaments (anterior cruciate ligament (ACL), posterior cruciate ligament (PCL), lateral collateral ligament (LCL) and medial collateral ligament (MCL)) have been carried out in the literature (Gardiner et al. 2001; Yoo et al. 2010; Aunan et al. 2012; Belvedere et al. 2012; Rochcongar et al. 2016; Pedersen et al. 2019). Although these studies have substantially increased knowledge on joint functions, yet the complexity of measurements, lesser availability of cadavers, ethical and cost implications have made data acquisition challenging.

Alternatively, finite element (FE) models are commonly used as a reliable complementary means to experimental studies providing significant insight into knee joint biomechanics. A variety of modeling techniques have been utilized to model the joint structure, particularly ligaments. Some of the strategies are steered by simplicity, while others concentrate on faithful capture of specimen-specific anatomy with varying levels of joint representation fidelity. For example, some models included 3D geometries of ligaments with complex material behavior (Limbert et al. 2004; Peña et al. 2005; Kiapour et al. 2014; Orsi et al. 2016). Such approach allows to consider ligament wrapping behavior and analysis of local biomechanical response (e.g., 3D stresses and strains across tissue). Nevertheless, higher anatomically complex models require detailed image-based information of the soft tissue structures under consideration. Generation and simulation of such models often require manifold higher time than that for

1  
2  
3 73 simpler models (Bolcos et al. 2018). Therefore, simpler models may be beneficial for studies  
4  
5 74 where higher number of subjects need to be analyzed and, at the same time, capable of  
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7  
8 75 predicting joint mechanics.

9  
10 76 In an attempt for model simplification, other authors have proposed to represent ligaments  
11  
12 77 as bundles of springs or tension only cables (Moglo and Shirazi-Adl 2005; Adouni and Shirazi-  
13  
14 78 Adl 2009; Baldwin et al. 2012). Although ligaments are exposed to both compressive and  
15  
16  
17 79 tensile states of stress, yet the contribution of tensile stress is substantially higher than others  
18  
19 80 (Peña et al. 2006; Orsi et al. 2016). Therefore, such simplification is considered reasonable and  
20  
21 81 recommended particularly for predicting joint kinematics (Naghibi Beidokhti et al. 2017).  
22  
23 82 Nevertheless, personalization of ligament properties (stiffness and prestrain), although  
24  
25 83 clinically essential to restore joint stability, yet represents a challenge for the community. For  
26  
27 84 example, there is a consensus that graft under-tensioning could lead to joint laxity, which is  
28  
29 85 biomechanically analogous to a ligament deficient knee (Sherman et al. 2012). In addition to  
30  
31 86 that, owing to variable morphology, different bundles of a ligament (e.g., two main fiber  
32  
33 87 bundles of ACL) may exhibit variable prestrain by becoming active at different flexion angles  
34  
35 88 (Girgis et al. 1975). From a modeling perspective, it has also been reported that incorrectly  
36  
37 89 applied ligament prestrain can have a considerable effect on the kinematics of the knee (Mesfar  
38  
39 90 and Shirazi-Adl 2006; Rachmat et al. 2016). To tackle this issue, some authors made subject-  
40  
41 91 specific adjustment using inverse methods to calibrate specific ligament constitutive behavior.  
42  
43 92 Models either used laxity tests (Baldwin et al. 2012; Naghibi Beidokhti et al. 2017) or  
44  
45 93 distraction loading (Zaylor et al. 2019) to estimate ligament properties by minimizing  
46  
47 94 differences between model-predicted and experimental kinetics. Such calibrations are,  
48  
49 95 however, likely to be computationally expensive.

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51 96 In light of the above considerations, we proposed an original framework for calibrating  
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53 97 subject-specific tensioning of FE knee ligaments based on experimentally acquired data.  
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3 98 Subject-specific model evaluation was performed by comparing predicted femorotibial  
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5 99 kinematics under passive flexion with the experimental data of six cadaveric specimens. We  
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7  
8 100 hypothesized that the employed methodology of building personalized FE models with  
9  
10 101 experiment-based prestrains could predict overall passive kinematics of the knee joint.

## 12 102 **2. Materials and methods**

14 103 The overall workflow of generating specimen-specific FE mesh is presented in figure 1

17 104 **[Figure 1 here]**

### 20 105 **2.1. Experimental data acquisition**

22 106 We obtained the experimental knee kinematic responses in a previous study (Rochcongar et al.  
23 107 2016). The experimental procedure is recalled briefly hereafter. Six fresh-frozen lower limb  
24 108 specimens harvested from subjects with age range 47 to 79 years, were tested under passive  
25 109 flexion-extension on a previously validated kinematic test-bench (Hsieh and Draganich 1997;  
26 110 Azmy et al. 2010). Skin and muscles were removed except eight centimeters of quadriceps  
27 111 tendon and popliteus muscle prior to the kinematic data collection. All other relevant joint soft  
28 112 tissue structures (such as ligaments, articular capsule) were kept intact during kinematic data  
29 113 acquisition. The femur was kept fixed, and flexion movement was introduced to the tibia by a  
30 114 rope and pulley system. During flexion, the positions of the three marker tripods placed on the  
31 115 femur, tibia, and patella were recorded using an optoelectronic system (Polaris, Northern  
32 116 Digital Inc., Canada). These recorded positions allowed establishing ancillary reference frames  
33 117 (referred to as  $R_{ANC_{POL}}(t)$ ) from  $t = 0$  (before applying flexion load) till the end of flexion  
34 118 (Figure 1(a)). Measurement uncertainties with the optoelectronic system was previously  
35 119 assessed. Overall uncertainties of less than 0.5 mm in translational and  $1^\circ$  in rotational DoF  
36 120 were obtained (Azmy et al. 2010).

37 121 In addition, two orthogonal radiographs of each specimen were acquired using an EOS  
38 122 biplanar X-ray system (EOS, EOS-imaging, France) to obtain 3D digital models of the bones

1  
2  
3 123 and tripod markers. From the 3D models, anatomical reference frames (referred to as  
4  
5 124  $R_{ANAT_{EOS}}$ ) for the femur, tibia, and patella were defined (Schlatterer et al. 2009). Ancillary  
6  
7  
8 125 reference frames (referred to as  $R_{ANC_{EOS}}$ ) from the tripod markers were also defined allowing  
9  
10 126 a relationship between anatomical frames and ancillary frames, termed as  $M_{ANAT_{ANC}}$   
11  
12 127 (Figure 1(b)). This relation was further used for converting acquired kinematic data,  $R_{ANC_{POL}}$   
13  
14  
15 128 ( $t$ ) to relative patellofemoral and tibiofemoral motions in the femur anatomical reference frame  
16  
17 129 with Cardan sequence  $ZY'X''$ .

20 130 After the kinematic data acquisition, each specimen was fully dissected to identify the  
21  
22 131 ligament attachment sites. Absence of trauma and integrity of soft tissue structures was checked  
23  
24 132 during the dissection. An experienced surgeon identified the origin and insertion locations for  
25  
26 133 the following ligaments: anteromedial (AM) and posterolateral (PL) bundles of ACL,  
27  
28 134 posteromedial (PM) and anterolateral (AL) bundles of PCL, superficial (MCLs) and deep  
29  
30 135 (MCLd) bundles of MCL, and LCL. Identified locations were marked with radio-opaque  
31  
32 136 paints, and the bones were scanned using a computed tomography (CT) scanner (Philips, Best,  
33  
34 137 The Netherlands). 3D digital models of each dissected specimen were acquired using MITK-  
35  
36 138 GEM (version 5.0) giving anatomical frames ( $R_{ANAT_{CT}}$ ) and ligament attachment sites ( $P_{LIGA_{CT}}$ )  
37  
38 139 in the CT scanner system of reference (Figure 1(c)). 3D Digital models and digital  
39  
40 140 footprints of ligament attachment sites were then registered into experimental initial  
41  
42 141 configuration. Registration was performed with biplanar X-ray data. Once the centroidal  
43  
44 142 coordinates of the attachment sites were known, the end-to-end distance of the ligaments origin  
45  
46 143 and insertion site was computed at experimental initial configuration. For the sake of  
47  
48 144 readability, end-to-end distance will be referred to as ligament length hereafter.

## 145 2.2. Initial bone pose estimation

1  
2  
3 146 Relative pose (position and orientation) of tibia and patella w.r.t. the femur at initial unloaded  
4  
5 147 configuration was obtained using the relation  $M_{ANAT\_ANC}$  and experimental kinematic data,  
6  
7  
8 148  $R_{ANC_{POL}}(t)$  at time=0 (Figure 1(d)).  
9

### 10 149 **2.3. Specimen specific FE model**

#### 11 150 *2.3.1. FE mesh*

12  
13 151 First, subject-specific FE hexahedral mesh for each bony segment was created based on the  
14  
15 152 subject-specific CT based digital models (Figure 1(e)) (Lahkar et al. 2018). Then, only the  
16  
17 153 surface mesh (4-noded shell element) was kept to represent bones and cartilage to reduce  
18  
19 154 computational cost (Germain et al. 2016). Then, mesh smoothing was performed at the articular  
20  
21 155 surfaces to improve the mesh quality (Taubin 1995).  
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26  
27 156 Mesh quality was assessed using standard ANSYS mesh quality indicators: aspect ratio,  
28  
29 157 parallel deviation, maximum angle, Jacobian ratio, and warping factor. The surface accuracy  
30  
31 158 of specimen specific mesh for each specimen was compared against respective 3D digital  
32  
33 159 model (i.e. segmented 3D geometry from CT data) by registering Hausdorff distance expressed  
34  
35 160 in mean (2RMS) values.  
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#### 39 161 *2.3.2. Knee joint FE model*

40  
41 162 Bones were assumed to be isotropic linear elastic with Young's modulus of 12000 MPa (Choi  
42  
43 163 et al. 1990). As the loading pattern in the study is quasi-static, cartilage was assumed as single-  
44  
45 164 phase linear isotropic material (Eberhardt et al. 1990). Cartilage regions were modeled as  
46  
47 165 cortico-cartilage material and assigned with Young's modulus of 250 MPa to summarize the  
48  
49 166 material properties of cortical bone and cartilage (Germain et al. 2016). A very thin strip of  
50  
51 167 material between bones and cortico-cartilage region were also modeled with intermediate  
52  
53 168 properties (2000 MPa) to limit mechanical discontinuity (Germain et al. 2016) (Figure 2).  
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57

58 169 **[Figure 2 here]**

1  
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3 170 Attachment sites for the cruciate and collateral ligaments were based on the already  
4  
5 171 identified locations (Rochcongar et al. 2016). For other ligaments and tendons (femoro-patellar  
6  
7 172 ligament, patellar tendon, quadriceps tendon, posterior capsule), general anatomical sites based  
8  
9 173 on *a priori* knowledge of an anatomist were used. Each cruciate ligament was represented by  
10  
11 174 2 bundles (Blankevoort and Huijkes 1991) along with MCL (deep and superficial) (Smith et  
12  
13 175 al. 2016). Posterior capsule and femoropatellar ligaments were each represented by 8 bundles  
14  
15 176 (4 bundles in the medial and lateral side each), while quadriceps and patellar tendon as 4  
16  
17 177 bundles each (Germain et al. 2016) and LCL as one (Meister et al. 2000). All ligaments and  
18  
19 178 tendons were represented as point-to-point, tension-only cable elements as their contribution  
20  
21 179 in tension is much higher than that in compression (Baldwin et al. 2009; Harris et al. 2016).  
22  
23 180 Three frictionless surface-to-surface contact pairs were considered: tibia-femur cartilage  
24  
25 181 (medial and lateral) and femur-patella cartilage with augmented penalty solution algorithm.  
26  
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### 33 183 2.3.3. Ligament material properties

34  
35 184 Three cases of ligament prestrain values ( $\% \epsilon$ ) were considered for cruciate and collateral  
36  
37 185 ligaments. No prestrain values for other ligaments were considered and stiffness ( $k$ ) values for  
38  
39 186 all the ligaments were adopted or estimated from our previous study (Germain et al. 2016). It  
40  
41 187 is to be noted that constant stiffness values were applied across all specimens.  
42  
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44

45 188 [Figure 3 here]

46  
47 189 **Case 1: Generic material properties.** Prestrain values for ACL (5%), PCL (-3%), MCL (0%)  
48  
49 190 and LCL (0%) were adopted from previous study (Germain et al. 2016).  
50

51  
52 191 **Case 2: Automatic pre-computation from experimental data.** For each specimen, ligament  
53  
54 192 and bundle specific prestrains were automatically computed from the experimental ligament  
55  
56 193 lengths using equation 1. This is illustrated for the MCL in figure 3.  
57

58  
59 194 **Case 3: Combination of automatic pre-computation and further manual adjustment.**  
60

1  
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3 195 Initial values for the 7 ligament parameters (prestrains) were assigned with  
4  
5 196 precomputed ligament prestrains. The minimum and maximum bounds for each parameter was  
6  
7 197 defined from the literature (Blankevoort and Huiskes 1996; Baldwin et al. 2009). Each  
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9  
10 198 parameter at a time was modified by changing the previously assigned value by roughly 10%  
11  
12 199 and RMS error between numerical and experimental kinematics was observed for each DOF.  
13  
14 200 Based on the error, a new parameter set was assigned. Thus the procedure was repeated till  
15  
16 201 rotational and translational RMS error became steady state. Stopping criteria was chosen as  
17  
18 202 change in RMS error between two consecutive iterations is less than or equal to 0.1° for  
19  
20  
21 203 rotational and 0.1 mm for translation.

$$24 \quad 204 \quad 25 \quad 205 \quad \text{prestrain} = \left(\frac{\delta}{L}\right) * 100 = \left(\frac{L - L_0}{L}\right) * 100 \quad (1)$$

26  
27  
28 206 where, L is the experimental ligament length at initial configuration (before application of  
29  
30 207 flexion load), and  $L_0$  is the zero-strain length at the end of flexion, with an assumption that  
31  
32 208 ligaments experience no force after the prescribed maximum flexion angle.

#### 33 209 2.3.4. FE model simulation states

34  
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37 210 Three different configurations were defined to represent different simulation states applicable  
38  
39 211 to all the FE models and all cases of ligament properties. As the models are built from the  
40  
41 212 experimental initial configuration, the first state is referred to as (a) **no-load or stress free**  
42  
43 213 **configuration**. The second state corresponds to the configuration after attaining equilibrium  
44  
45 214 under prestrain effect, termed as (b) **initial equilibrium configuration** (or reference  
46  
47 215 configuration). The third state corresponds to the deformed states of the model upon application  
48  
49 216 of incremental rotational displacements on the tibial malleolus until 70° of flexion angle  
50  
51 217 (Germain et al. 2016). Knee flexion took place at the third state and referred to as (c) **current**  
52  
53 218 **deformed configuration**. Remaining DOFs were left unconstrained. Only geometric non-  
54  
55 219 linearity was considered for the model simulations.

220 *2.3.5. Model evaluation: Knee joint kinematics*

221 The relative position and orientation of the tibia w.r.t. femur was computed based on their  
222 anatomical reference frames, as described in (Schlatterer et al. 2009) and interpreted in the  
223 femur anatomical reference frame. One-to-one model evaluation was performed by comparing  
224 predicted femorotibial kinematics to experimental measurements throughout flexion motion  
225 for both the cases 2 and 3. Specimen specific RMS differences between model-predicted and  
226 experimental measurements were computed based on values at 1° interval for a range of flexion  
227 angle 0–60°. Eventually, RMS difference with experimental data was averaged for all the  
228 specimens.

229 **3. Results**

230 *3.1. Mesh quality*

231 Quality of individual knee joint FE mesh showed no occurrence of error in terms of ANSYS  
232 mesh quality indicators.

233 *3.2. Surface representation accuracy*

234 [Figure 4 here]

235 FE mesh surface accuracy for the femur, tibia, and patella w.r.t. corresponding CT surface  
236 across all specimens were found less than or equal to (mean (2RMS) in mm) 0.04 (0.12), 0.06  
237 (0.18) and 0.05 (0.14) respectively. Error-values are pictorially represented in figure 4 for  
238 specimen 1 for the sake of example.

239 *3.3. Estimation of subject-specific ligament material properties*

240 *3.3.1. Case 2: Based on automatic pre-computation from experimental data*

241 [Table 1a and Table 1b here]

242 Estimated ligament stiffness and pre-strain values computed according to the procedure  
243 described in subsection 2.3.3 (case 2) are presented in Table 1a and Table 1b, respectively.

244 Positive prestrain denotes tight condition and negative prestrain slack condition. Ligament  
245 prestrains showed both ligament-specific and specimen-specific variability.

### 246 3.3.2. Case 3: Combination of automatic pre-computation and further manual adjustment

247 **[Table 1c here]**

248 Estimated ligament pre-strain values computed according to the procedure described in  
249 subsection 2.3.3 (case 3) are presented in Table 1c. Ligament stiffness values were kept the  
250 same as presented in Table 1a.

### 251 3.4. One-to-one validation of knee joint kinematics

252 On implementation of the generic ligament properties (case 1), only two FE models out of six  
253 achieved full convergence. **Convergence in this study refers to successful attainment of**  
254 **mechanical equilibrium (within a default tolerance value of ANSYS) at each load step.**

255 Predicted kinematics showed large deviation from the experimental both in magnitude and  
256 trend (**not reported in this manuscript as only two models achieved convergence**). Using the  
257 ligament material properties computed automatically (case 2, Table 1b), 5 models out of 6  
258 achieved convergence throughout 60° of flexion.

259 **[Figure 5 and Figure 6 here]**

260 Using the ligament material properties computed automatically combined with manual  
261 adjustment (case 3, Table 1c), all the FE knee models remained stable throughout the range of  
262 flexion. Individual run time was approximately 13 minutes per specimen. One-to-one  
263 comparison of model predicted femorotibial kinematics against corresponding *in vitro* results  
264 for all specimens are presented in **Figure 5 and Figure 6 for automatically computed prestrains**  
265 **and adjusted ligament prestrains respectively**. For both the cases, model kinematics for all DOF  
266 are shown from the reference configuration (state-b) until the end of flexion movement.

267 **[Table 2 here]**

1  
2  
3 268 Table 2 summarizes the RMS difference between model-predicted and experimental  
4  
5 269 kinematics for the range of flexion angle 0–60° for the two cases (case 2 and case 3) of ligament  
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7 270 material properties. Since 5 models out of 6 were converged while applying automatically  
8  
9 271 computed ligament prestrains, differences are presented for 5 models.

#### 12 272 4. Discussion

14 273 Subject-specific tensioning of ligaments is essential in developing personalized knee FE  
15  
16 274 models. In this study, we built subject-specific knee FE model with CT-based geometry and  
17  
18 275 evaluated a new procedure for subject-specific calibration of ligaments prestrain from biplanar  
19  
20 276 X-ray data. Predicted femorotibial kinematics of each model was compared to the  
21  
22 277 corresponding *in vitro* response for three different cases of ligament properties (prestrain).  
23  
24 278 First, we investigated whether the FE models with generic prestrain values can capture inter-  
25  
26 279 individual variability of the *in vitro* kinematics. Second, experimentally obtained prestrains  
27  
28 280 were recruited to the FE models and predicted kinematics were observed (case 2). Third, model  
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30 281 kinematics were observed with respect to calibrated ligament properties based on the  
31  
32 282 combination of pre-computed prestrains and further adjustment (case 3). For case 2, RMS  
33  
34 283 differences between model-predicted and experimental results for abduction/adduction and  
35  
36 284 external/internal rotation were less than or equal to 2.4° and 6.3° respectively. For translation  
37  
38 285 kinematics, the differences observed were less than or equal to 5.0 mm, 1.9 mm and 1.2 mm  
39  
40 286 respectively for posterior/anterior, superior/inferior, and lateral/medial motions. For case 3,  
41  
42 287 improvement in model kinematics was observed with RMS differences 1.5° and 5.3° for  
43  
44 288 abduction/adduction and external/internal rotation. Differences for posterior/anterior,  
45  
46 289 superior/inferior, and lateral/medial motions were 3.4 mm, 1.2 mm and 2 mm respectively.  
47  
48 290 These results show that the proposed methodology allows us to obtain a good first  
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50 291 approximation of the prestrain values with further manual adjustment to improve the kinematic  
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52 292 prediction.  
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3 293 As far as the authors are aware of, there are numerous challenges exist in determining  
4  
5 294 ligament prestrain. Challenges are linked to both measurement issues and modeling issues.  
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7  
8 295 Measurement challenges are mainly methodological issues related to identification of ligament  
9  
10 296 attachment sites and determination of ligament elongation pattern during motion (Woo et al.  
11  
12 297 1990; Gardiner et al. 2001; Belvedere et al. 2012). Because of such difficulties, FE models in  
13  
14 298 general, adopt prestrain values from other studies available in the literature (Yang et al. 2010;  
15  
16 299 Galbusera et al. 2014). As these values are adopted from other experimental studies and not  
17  
18 300 corresponding to the specimen under consideration, thereby cannot be considered as subject-  
19  
20  
21 301 specific. Optimization methods have also been extensively used to calibrate specific ligament  
22  
23 302 constitutive behavior. These approaches particularly used laxity tests to calibrate their models  
24  
25 303 (Baldwin et al. 2012; Naghibi Beidokhti et al. 2017). Such approaches are, although shown  
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27 304 effective to attain specimen-specific ligament properties, yet computationally expensive.  
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30  
31 305 The current study focused on the development and evaluation of a new procedure for  
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33 306 subject-specific tensioning of FE knee ligaments. The proposed procedure builds upon data  
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35 307 previously collected during an experimental investigation conducted to identify ligament  
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37 308 (cruciate and collateral) attachment sites, and to determine the ligament elongation patterns  
38  
39 309 during passive knee flexion (Rochcongar et al. 2016). The FE model replicates the natural  
40  
41 310 ligament (cruciate and collateral) insertions since these are derived from the radio opaque paint  
42  
43 311 locations painted on the specimens prior to the CT-scan (figure 1). The values obtained were  
44  
45 312 consistent with those experimental measurements reported in the literature (Bicer et al. 2010;  
46  
47 313 Belvedere et al. 2012). It is worth mentioning that because of the lack of experimental data for  
48  
49 314 other ligaments, generic insertion sites were employed. Although, it is difficult to directly  
50  
51 315 compare the estimated prestrains with similar studies in literature because of variability in  
52  
53 316 ligament geometry and material property, yet the prestrain values were found within the range  
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55 317 confirmed by others (Wismans et al. 1980; Amiri et al. 2006; Zaylor et al. 2019). Also, most  
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3 318 of the ligaments were found in tensed state at full extension except PCL, which is overall in  
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5 319 agreement with the literature (Blankevoort and Huijkes 1991; Moglo and Shirazi-Adl 2005;  
6  
7 320 Guess et al. 2016). Similarly, predicted kinematic response also showed good correspondence  
8  
9 321 with the experimental results for all specimens. The experimental-numerical differences found  
10  
11 322 in this study were comparable to similar studies reported in the literature (Harris et al. 2016;  
12  
13 323 Naghibi Beidokhti et al. 2017). For instance, Beidokhti et al. reported an average RMS  
14  
15 324 difference of 3.5° and 2.8° respectively for abduction/adduction and external/internal rotations.  
16  
17 325 For anterior/posterior, superior/inferior and lateral/medial motions the differences were 3 mm,  
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19 326 2.3 mm and 1.6 mm respectively. It is worthwhile to mention that when generic properties were  
20  
21 327 used, most of the models couldn't reach convergence. As previously reported by other research  
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23 328 teams (e.g., (Schwartz et al., 2019)) focusing on the medial collateral ligament) convergence  
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25 329 difficulty appeared in this kind of models when material properties were not personalized.

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31 330 The procedure to compute ligament prestrain directly from experimental data (Case 3)  
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33 331 provided satisfactory initial guess, based on which model estimated kinematics were already  
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35 332 in good agreement with the experimental data. As this approach appears to be computationally  
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37 333 inexpensive (15-20 sec to obtain ligament specific prestrain for a single knee model) and  
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39 334 methodologically simple, it may serve as a reliable alternative for estimating subject-specific  
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41 335 ligament prestrain values. To be noted that no direct evaluation of the ligament tensions was  
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43 336 performed in the present study. The decision to implement the current technique as an  
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45 337 alternative has to be conducted with caution. For successful implementation of this technique  
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47 338 towards clinics, exhaustive model evaluation under various loading conditions is required  
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49 339 including ligament tension and contact stress. Nevertheless, validating joint kinematics as a  
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51 340 first step could be valuable to show feasibility of the current approach.

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56 341 This study contains some considerations and limitations worth highlighting. **First**,  
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58 342 while comparing with experimental kinematics, model-predicted results were shown from  
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3 343 reference configuration (state-b). It is an auto-equilibrated configuration under the prestrain  
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5 344 effect, which is not concurrent with initial experimental configuration and difficult to calibrate.  
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8 345 This results in absolute offset from the experimental kinematics (Baldwin et al. 2012), although  
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10 346 masked in relative kinematics. **Second**, we acknowledge that one of the sources of  
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12 347 discrepancies between experimental-numerical kinematics may come from model  
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14 348 simplifications and assumptions. **It is also to be noted that predicted kinematics with a**  
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16 349 **combination of initial guess from experimental data and further manual adjustment displayed**  
17  
18 350 **closer correspondence to *in vitro* data.** Although the difference is minimal, this may be  
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20 351 attributed to the representation of overall joint soft tissue structure with simple ligamentous  
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22 352 structures without including cartilage layers and menisci. **As the proposed methodology is not**  
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24 353 **based on current state-of-the-art approaches (such as MRI based complex models with detailed**  
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26 354 **soft tissue structures), there was difficulty to obtain subject-specific geometry of cartilage and**  
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28 355 **menisci with available imaging modalities (CT and biplanar X-ray) employed in our study.**  
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31 356 Such simplification, therefore doesn't hold if we are interested in more detailed local insights,  
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33 357 e.g., cartilage contact stress. However, for analysis, such as graft tensioning effect on knee  
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35 358 response while reconstructing ACL, such simplification was considered relevant (Peña et al.,  
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37 359 2005). **Third**, exclusion of meniscus may overestimate the role of the ligaments in constraining  
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39 360 the joint and providing stability (Harris et al. 2016). However, other studies reported no  
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41 361 remarkable influence of meniscus on the assessment of the knee joint kinematics, especially  
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43 362 for the flexion range 0°–90° (Amiri et al. 2006; Guess et al. 2010). **Fourth**, ligaments and  
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45 363 tendons were represented as bundles of 1D elements, which may not capture actual ligament  
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47 364 length variation, as they do not account for material continuum, fiber twisting or wrapping.  
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49 365 Yet, such simplification provides faster solutions and recommended, particularly for **the**  
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51 366 **prediction of knee kinematic parameters** (Bolkus et al., 2018; Naghibi Beidokhti et al., 2017).  
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54 367 **Fifth**, we chose to personalize only ligament prestrains, although stiffness values vary from  
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3 368 subject to subject. This consideration was based on sensitivity analyses found in literature,  
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5 369 where model predicted kinematics are proclaimed to be highly sensitive to strain state at initial  
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7 370 configuration rather than stiffness values (Wismans et al. 1980; Peña et al. 2005). Besides, the  
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9 371 models were validated only under passive flexion load, which may not imitate an in-vivo  
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11 372 situation of clinical interest, yet could be a first step of assessing the potential of the models  
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13 373 towards complex scenarios. In this contribution, a maximum flexion angle of 70° was  
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15 374 considered to calibrate the model as this range covers the most common amplitude of in-vivo  
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17 375 motion under level walking, during which ligaments offer a substantial contribution to knee  
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19 376 stability (Butler et al. 2007). However, perspective work will focus on calibrating the model  
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21 377 up to 120° of knee flexion. We acknowledge that no influence of experimental uncertainty nor  
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23 378 sensitivity of ligament attachment sites on predicted kinematics was performed. Future study  
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25 379 is necessary to asses this issue. Finally, the study was limited to six specimens due to time and  
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27 380 labor associated with CT segmentation, yet higher in number compared to other similar  
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29 381 published studies. This might limit the model at the current state for clinical translation;  
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31 382 however, it was imperative to build CT based models to minimize the impact of geometrical  
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33 383 uncertainty in model predictions.

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35 384 In conclusion, as it was a first study to directly implement prestrain values on models  
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37 385 directly from the experiment, which may find scopes in model-based clinical studies, such as  
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39 386 planning of ligament balancing or reconstruction as it reduces complexity in model  
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41 387 development (especially ligament calibration) as well as computational cost, while maintaining  
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43 388 good correspondence with experimental data. In that aim, further model evaluation would be  
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45 389 necessary for larger specimen size and in other clinically relevant scenarios.  
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### 391 **Conflict of Interest**

392 None

## 393 Acknowledgments

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395 musculoskeletal modeling for financial support.

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## 526 Figure Captions

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31 528 **Figure 1.** Schematic illustration for (a) kinematic test: position of tripod markers in Polaris coordinate  
32 529 system (CSYS), (b) biplanar X-ray: 3D digital models of bone and tripod markers giving anatomical  
33 530 and ancillary reference frames in EOS CSYS, (c) CT scan: Accurate 3D digital models of bone and  
34 531 ligament attachment sites giving anatomical reference frames and ligament attachment locations in CT  
35 532 CSYS, (d) knee in experimental initial configuration giving anatomical reference frames in Polaris  
36 533 CSYS, (e) CT based subject-specific FE mesh and ligament attachment sites in experimental initial  
37 534 configuration  
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40 535 **Figure 2.** FE model with soft tissues (only shown for the distal femur and proximal tibia region)  
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43 536 **Figure 3.** Experimental ligament length change for superficial MCL throughout the flexion movement.  
44 537 A similar strategy was implemented for other ligaments except for PCL, which is based on literature  
45 538 values  
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47 539 **Figure 4.** Surface representation accuracy as a Hausdorff distance for femur, tibia, and patella  
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49 540 **Figure 5.** One-to-one comparison of FE model kinematic predictions against corresponding  
50 541 experimental data for (a) – (b): rotational and for (c) – (e): translational femorotibial kinematics  
51 542 interpreted in femur anatomical reference frame. Results reported are based on the implementation of  
52 543 automatically computed ligament prestrains  
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55 544 **Figure 6.** One-to-one comparison of FE model kinematic predictions against corresponding  
56 545 experimental data for (a) – (b): rotational and for (c) – (e): translational femorotibial kinematics  
57 546 interpreted in femur anatomical reference frame. Results reported obtained using a combination of  
58 547 automatic pre-computation and further manual adjustment  
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3 549 **Table Headings**

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6 551 **Table 1a** Estimated ligament stiffness values for a single specimen

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8 552 **Table 1b** Automatically computed ligament prestrain values from experimental data (case 2)

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10 553 **Table 1c** Prestrain obtained with a combination of automatic pre-computation and further manual  
11 adjustment (case 3)

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14 555 **Table 2** Average RMS difference  $\pm$  SD between experimental and model-predicted kinematics

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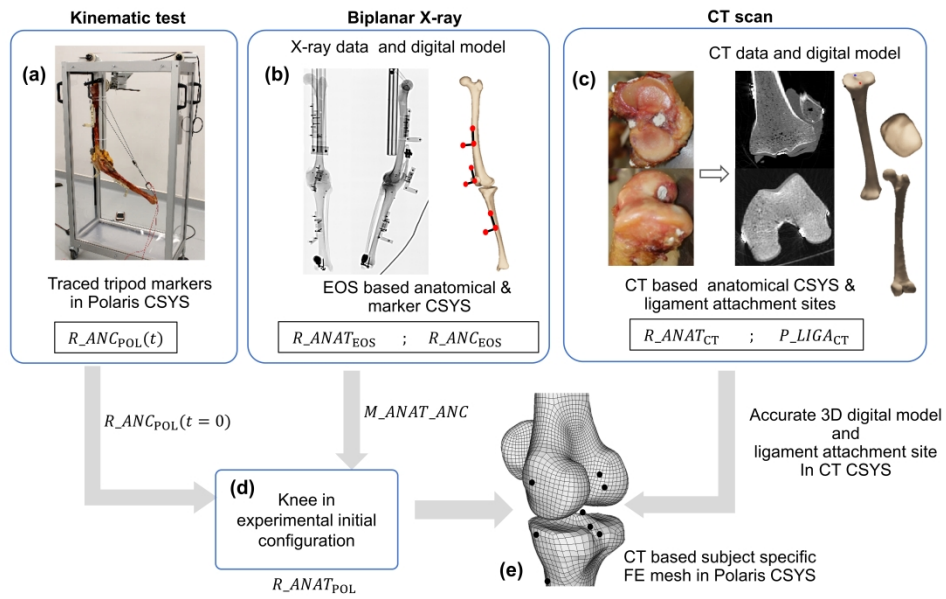


Figure 1

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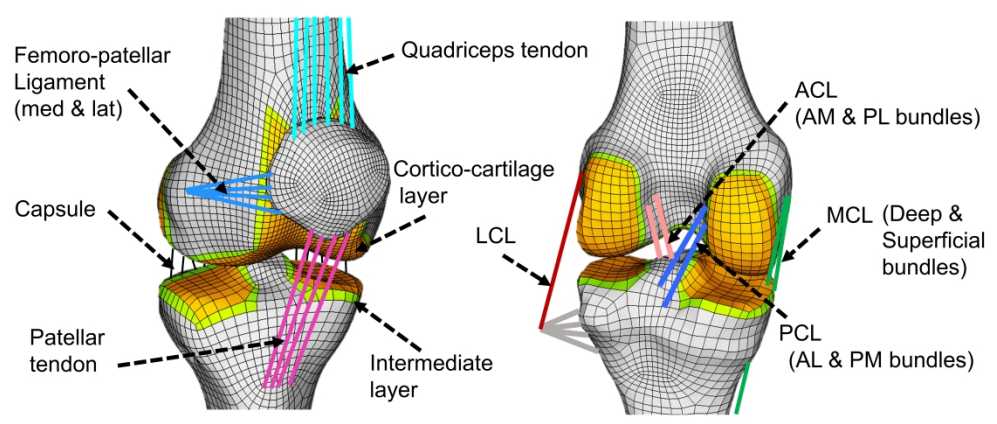


Figure 2

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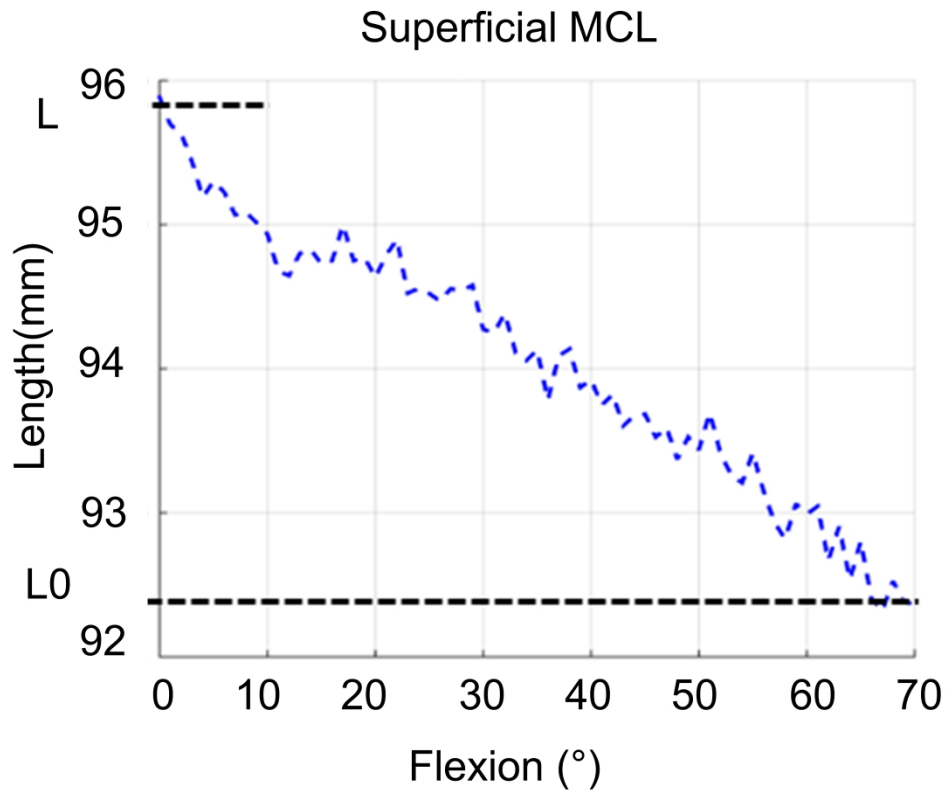


Figure 3

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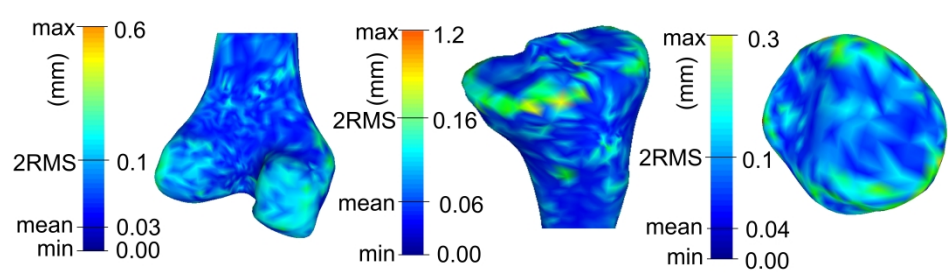


Figure 4

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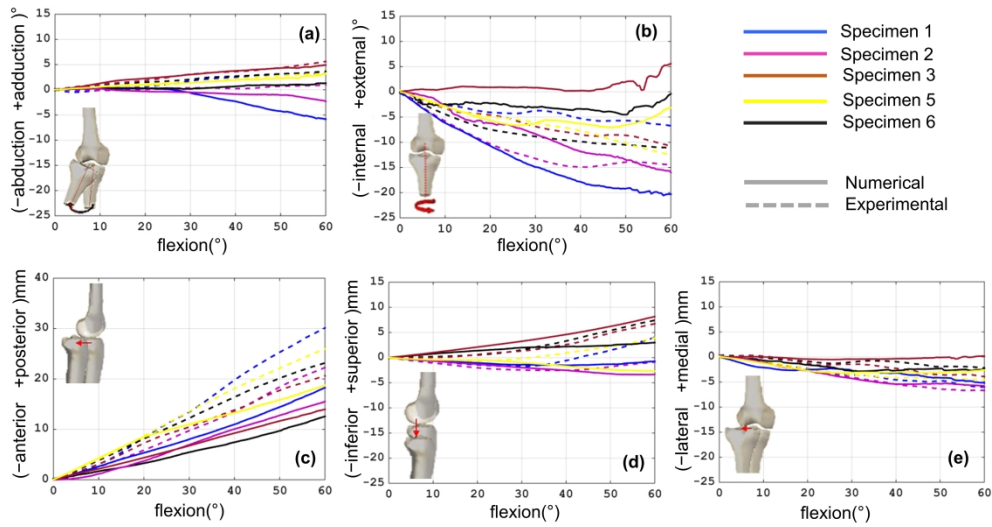


Figure 5

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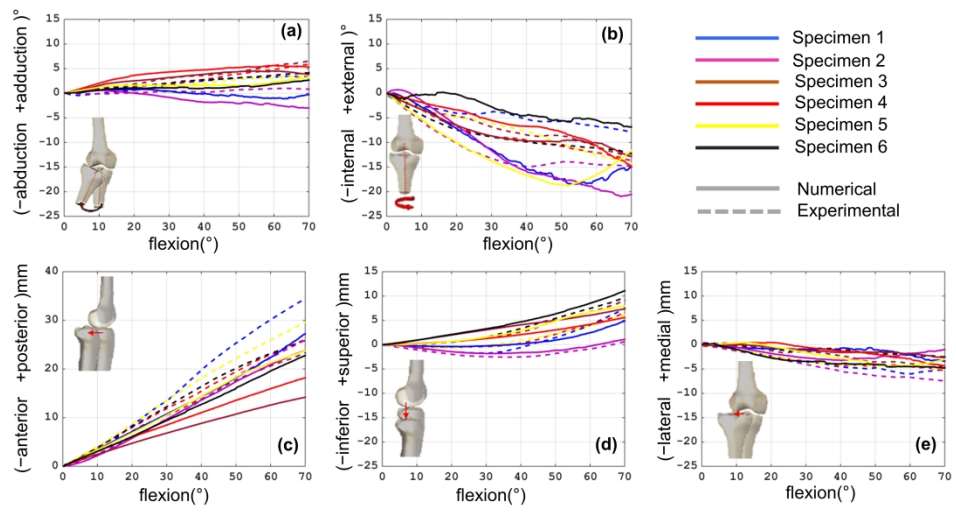


Figure 6

239x134mm (600 x 600 DPI)

**Table 1a**

Ligaments	ACL		PCL		MCL		LCL
Bundles	AM	PL	AL	PM	MCLd	MCLs	
Stiffness(N/mm)	125	105	125	65	45	25	60

**Table 1b: Case 2**

Specimens	ACL		PCL		MCL		LCL
	AM	PL	AL	PM	MCLd	MCLs	
Specimen1	8	14	-8	-20	-1	-3	10
Specimen2	6	17	-17	-3	10	5	10
Specimen3	-8	16	-10	-10	3	2	8
Specimen4	4	20	-16	-15	6	2	10
Specimen5	9	20	-15	-6	8	4	7
Specimen6	0	13	-9	4	-3	-2	9

Prestrain (%)

**Table 1c: Case 3**

	Ligaments & Bundles	ACL		PCL		MCL		LCL
		AM	PL	AL	PM	MCLd	MCLs	
Prestrain (%)	Specimen1	8	10	-2	-8	8	3	6
	Specimen2	6	12	-8	-4	6	3	5
	Specimen3	8	10	-8	-8	2	1	4
	Specimen4	10	10	-9	-5	2	3	6
	Specimen5	10	13	-5	-5	3	2	2
	Specimen6	6	6	-3	-3	4	3	3

**Table 2**

Flexion	Case	Abd/Add in°	Ext/Int in°	Post/Ant in mm	Sup/Inf in mm	Lat/Med in mm
	1	-	-	-	-	-
0 – 60°	2	2.4 ± 1.3	6.3 ± 6.2	5.0 ± 3.5	1.9 ± 1.8	1.2 ± 1.1
	3	1.5 ± 1.3	5.3 ± 5.1	3.4 ± 2.3	1.2 ± 0.8	2.0 ± 1.9