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## Introduction

Passive knee flexion is guided by the interaction of the articulating cartilage surfaces, ligaments, and menisci. Together these structures provide a large range of flexion/extension [1] and allow subtle coupled motions [2–4]. Treating ligament injury or joint degeneration with ligament reconstruction or joint replacement, respectively, relies on generating loading patterns in the reconstructed or remaining passive restraints that allow passive flexion with minimal resistance. Thus, surgeons often evaluate the range of flexion as a critical peri- and intra-operative assessment of knee function. Failure to restore loading patterns in the passive restraints may result in clinical complications that contribute to

# A Multibody Knee Model Corroborates Subject-Specific Experimental Measurements of Low Ligament Forces and Kinematic Coupling During Passive Flexion

A multibody model of the knee was developed and the predicted ligament forces and kinematics during passive flexion corroborated subject-specific measurements obtained from a human cadaveric knee that was tested using a robotic manipulator. The model incorporated a novel strategy to estimate the slack length of ligament fibers based on experimentally measured ligament forces at full extension and included multifiber representations for the cruciates. The model captured experimentally measured ligament forces ( $\leq 5.7N$  root mean square (RMS) difference), coupled internal rotation ( $\leq 1.6 \text{ deg}$  RMS difference), and coupled anterior translation ( $\leq 0.4 \text{ mm}$  RMS difference) through 130 deg of passive flexion. This integrated framework of model and experiment improves our understanding of how passive structures, such as ligaments and articular geometries, interact to generate knee kinematics and ligament forces.

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joint degeneration following ligament reconstruction or undesirable performance of joint replacements [5,6].

Computational models of the knee are hindered in their ability to predict kinematics and ligament loading patterns over a large range of flexion [7–12]. This limitation is related to three factors: (1) the choice of ligament slack length, defined as the length at which the ligament fibers begin to carry force; (2) the location and number of fibers used to represent the ligaments, especially the cruciates; and (3) failure to support the choice of these critical modeling parameters via subject-specific assessment of both knee kinematics and ligament forces (kinetics).

Ligament slack length has a strong effect on predictions of kinematics [8,13] and ligament forces [9] in computational models of the knee. However, previous methods for estimating this parameter have not been corroborated against subject-specific in situ forces in individual ligaments. Thus, it is not known whether the assumed slack length yields realistic ligament forces. This is a critical limitation since slack length could compensate for

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structures that were not modeled, such as the menisci [11,14,15] and capsular ligaments, leading to abnormally high ligament forces [16]. In previous studies, slack length was estimated by optimizing to the passive force–displacement response of the knee [8,17,18]; however, the predicted ligament forces were either not reported or not compared with experimental data. Other investigators imposed ligament pretension at full extension [9], which resulted in ligament forces that were higher than in situ measurements [19,20]. Ligament slack length was also previously determined via estimations based on ligament properties [21] or manual tuning [22], but no assessment of predicted forces against corresponding experimental measurements was reported.

The cruciate ligaments consist of multidirectional fiber bundles that provide restraint to the knee in multiple planes [23,24]. Previous investigators concluded that six to ten fibers are needed to model this multidirectional restraint [23,25], but many computational models employ a two-bundle formulation for the cruciates [11,21,26–28] based on their common clinical description [29,30]. However, this two-bundle formulation was incapable of reproducing experimentally measured force patterns from midflexion (60 deg) to deeper flexion (90–140 deg) [12]. This formulation also failed to predict a series of unidirectional subfailure tensile tests of the anterior cruciate ligament (ACL) in which the relative orientation of the insertions was varied [25]. These shortcomings suggest that the representation of the cruciates over a large range of flexion must better reflect their fiber architecture (i.e., fiber position and orientation) [23,24,31,32].

Therefore, we sought to: (1) integrate multibody dynamic modeling with subject-specific experimental measurements to estimate ligament slack length; (2) include formulations for the fiber architecture of the cruciate ligaments that reflect their anatomy; and (3) compare predictions of kinematics and ligament forces generated during passive knee flexion with subject-specific experimental measurements from full extension to deep flexion (130 deg). We hypothesized that the resulting model would capture two important features characteristic of passive knee flexion: (1) low ligament forces and (2) coupled internal rotation and anterior translation of the tibia.

#### Methods

**Experimental Procedure.** Using a robotic testing system [33], an in vitro physical experiment was conducted prior to developing the computational model. This physical experiment yielded data to assess predictions of the computational model on a one-to-one basis (Fig. 1).

Cadaver Knee Preparation and Imaging. A 20 yr old male right cadaver knee was used. The specimen was stored at -20 °C and thawed for 24 hrs at room temperature prior to testing. All the soft tissues 10 cm from the joint line were removed from the shafts of the femur, tibia, and fibula. Surrounding skin and musculature except for the popliteal muscle tendon complex were subsequently removed. All the remaining ligaments were left intact.

An L-shaped reference frame (L-frame) made of poly(methyl methacrylate) was rigidly attached to both the femur and the tibia via two #10-24 Delrin screws that were 2.5 cm in length. The L-frames allowed registration of the robotic experiment and the computational model (Fig. 2). Two perpendicular lines were etched on the surface of each arm of the L-frame. Two radiopaque glass tubes ( $\sim$ 55 mm in length and 5 mm in diameter) were embedded in each arm of the L-frame and were aligned parallel to the etched lines.

The knee was then placed in a computed tomography (CT) scanner (Biograph mCT, Siemens, Erlangen, Germany), positioned in full extension, and scanned axially with a slice thickness of 0.625 mm and in-plane pixel dimensions of  $0.6 \times 0.6 \text{ mm}^2$ . The CT data were subsequently used to generate 3D models of the femur, tibia, fibula, and the glass tubes embedded in the L-frames. Each glass tube was represented with about 3000 points. Principle component analysis (PCA) was used to identify the direction vectors corresponding to the long axes of these points. The direction



Fig. 1 Flowchart summarizing the model development procedure (dashed gray box) and subject-specific comparison of model predictions with the physical experiment

vectors were used to define a homogeneous transformation matrix. The origin of this transformation matrix was the midpoint of the shortest distance between the two direction vectors.

After imaging, the specimen was inspected via direct medial parapatellar arthrotomy to assure that no signs of ligamentous deficiency, bony abnormalities, or articular degeneration were present. The fibula was then cut about 6 cm from its proximal end and fixed to the tibia using a wood screw to maintain its anatomical orientation. The femur and tibia were potted in bonding cement (Bondo, 3M, St. Paul, MN). Four wood screws were drilled transversely along the length of the tibial and femoral shafts to ensure fixation between the bone and cement.

Physical Experiment of Passive Flexion. The specimen was mounted to a six degrees-of-freedom robot (ZX165U, Kawasaki Robotics, Wixom, MI) instrumented with a universal force/ moment sensor (resolution:  $F_x = F_y = 0.125$  N,  $F_z = 0.25$  N,  $T_x = T_y = T_z = 0.0075$  N·m, Theta, ATI, Apex, NC) mounted to the robot's end effector. The potted femur was first fixed to a pedestal that was secured to the floor and then the knee was visually aligned in full extension. The tibia was subsequently mounted to a fixture attached to the end effector of the robot.

The locations of anatomical landmarks on the tibia and femur were identified with the knee mounted to the robot at full extension using a 3D digitizer with  $\leq 0.05$  mm accuracy (MicroScribe MX, Solution Technologies, Inc., Oella, MD). The landmarks included: the femoral epicondyles, the distal tibia, the fibular insertion of the lateral collateral ligament (LCL), and a point in the center of the superficial medial collateral ligament (sMCL) about 15 mm below the joint line. These landmarks were subsequently used to define bone-fixed coordinate systems for the tibia and femur [33]. The position and orientation of the tibia relative to the femur were expressed by adapting the conventions defined by Grood and Suntay [33,34]. All the translations were referenced to the midpoint of the line connecting the femoral epicondyles.

The L-frames were subsequently identified by using the 3D digitizer to scribe the two lines etched on the surface of each Lframe. The location of the digitizer was kept constant across the entire digitization process. This enabled the L-frames to be located relative to the previously digitized anatomical landmarks.





Fig. 2 L-frames were rigidly fixed to the tibia and femur and identified using a 3D digitizer after the knee specimen was mounted to the six degrees-of-freedom robot in full extension

Digitization of each etched line yielded about 100 points. The major axis of each set of points was identified using PCA. This yielded two direction vectors for each L-frame, which were used to define a homogeneous transformation matrix in the same manner as previously defined for the CT data of the glass tubes. The homogeneous transform defined by the etched lines was parallel and offset by a fixed amount (5.75 mm) with respect to the homogeneous transform defined by the glass tubes.

Next, the path of passive flexion was determined from full extension to 130 deg flexion in 1 deg increments. This path was defined as the position and orientation of the tibiofemoral joint that achieved 10 N compression with zero forces and moments in the remaining directions within resultant loads of 5 N and  $0.4 \text{ N} \cdot \text{m}$ . A load-minimization algorithm based on a Newton–Raphson method [35] was implemented using custom code (MATLAB, MathWorks, Natick, MA) to identify the kinematic trajectory that minimized the difference between the current and targeted knee load.

The in situ forces borne by the ligaments were measured across the entire flexion path by serially sectioning each structure and using the principle of superposition [36]. The ligaments were identified and sectioned by a fellowship-trained orthopedic surgeon. The in situ ligament forces were determined for the ACL, posterior cruciate ligament (PCL), the sMCL, the central arm of the posterior oblique ligament (POL) [37], the medial- and lateral-posterior capsule (MPC and LPC, respectively), the fabellofibular ligament (FFL) [38], and the LCL. The experimentally measured knee forces were filtered using a fourth-order Butterworth low-pass filter with a 0.1 Hz cut-off frequency. The cut-off frequency was selected to be 1/6th of the highest frequency in the force data to eliminate high frequency components of the signal. The filter was implemented using the signal processing toolbox available in MATLAB.

*Cartilage and Meniscal Imaging.* The disarticulated tibia and femur with overlying articular cartilage and the menisci were CT-scanned after the physical experiment was completed. The procedure was devised to achieve a composite image of these three tissues. The bones and menisci were first dissected of remnants of any other soft tissues. Subsequently, the disarticulated tibia and femur were aligned sagittally in the core of the CT and scanned (0.625 mm slice thickness,  $0.6 \times 0.6 \text{ mm}^2$  in-plane pixel dimensions). After this scan was completed, the menisci were positioned anatomically on top of the tibia and sutured to the tibia at their horn attachments. The tibia and menisci were then scanned sagittally, producing a composite image of the tibial bone, cartilage, and meniscal geometries.

#### **Model Development**

Knee Geometries and Ligament Insertions. The CT images were imported into image processing software (Mimics, Materialise, Inc., Leuven, Belgium). The bone and cartilage geometries were isolated in two steps. First, using gray level thresholding, a mask was generated for the bone and for the combined geometry of the bone and cartilage. Then, Boolean subtraction was used to isolate the cartilage geometries (Fig. 3(a)). Similarly, the meniscal geometries were identified by overlapping a mask of the combined geometries of the tibia, cartilage, and menisci with the mask containing only the geometries of the tibia and the cartilage. Subsequently, Boolean subtraction was used to isolate the meniscal geometries (Fig. 3(b)). The surfaces were then smoothed using a filtering feature (remove spikes) available in Geomagic Studio (Geomagic, Inc., Morrisville, NC), which detected and flattened single-point spikes on the surface mesh.

The insertions of the fibers used to represent each ligament were obtained from the CT images, from dissecting the specimen, and from the literature [30,37-43] (Figs. 4(a)-4(f)). The ACL consisted of six fibers (Fig. 4(a)) with the tibial insertions of the fibers divided into anteromedial (AM), anterolateral (AL), and posterolateral (PL) groups based on the description by Butler et al. [44]. The femoral insertions of the fibers were placed halfway between the lateral intercondylar ridge (i.e., resident's ridge) and the posterior femoral cartilage [31,32,45,46]. The three most proximal femoral insertions were connected to the AM and AL insertion groups on the tibia. The three most distal femoral insertions were based on the fiber-level dissection of the ACL by Hara et al. [24].

The PCL was represented with seven fibers (Fig. 4(b)). The tibial insertions of the PCL fibers were divided into AL and posteromedial (PM) groups [40]. The femoral insertions were located along the medial intercondylar ridge [39]. The four insertions closest to the posterior cartilage on the lateral aspect of the medial femoral condyle were connected to the PM group of tibial insertions. The three insertions closest to the top of the femoral notch were connected to the AL group of tibial insertions.

The sMCL was divided into distal and proximal groups consisting of three fibers each (Fig. 4(*c*)). The POL, MPC, and LPC were each described by three fibers spanning the area that they cover [38] (Figs. 4(*c*) and 4(*d*)). The oblique popliteal ligament (OPL) was divided into posterior and distal fibers [38] (Fig. 4(*e*)). The LCL, the anterolateral ligament (ALL), and the FFL were each represented with one fiber (Fig. 4(*f*)) [38,43]. The horn attachments of the medial and lateral menisci were also modeled with one fiber each (Fig. 5). Seven fibers represented the attachments of the coronary ligaments from the medial meniscus to the tibial plateau (Fig. 5(*a*)). The lateral coronary ligament was represented with one fiber (Fig. 5(*b*)).

All the knee geometries and ligament insertions were transformed using the L-frames to the femoral coordinate system defined in our robotic experiments (see Appendix A). The



Fig. 3 Boolean subtraction was used to develop 3D geometries of (a) the tibial and femoral (not shown) articular cartilage and (b) the menisci. The surfaces were subsequently smoothed.



Fig. 4 Fibers representing the ligaments in the multibody model: (a) ACL (six fibers), (b) PCL (seven fibers), (c) sMCL (three proximal fibers and three distal fibers), POL (three fibers), (d) MPC and LPC (three fibers each), (e) OPL (two fibers), (f) FFL (one fiber), LCL (one fiber), and ALL (one fiber)

maximum error of the method was 0.60 mm in the medial-lateral direction and 0.17 deg about the internal-external rotation axis. This process enabled use of a common anatomical coordinate system to compare the kinematics measured in the physical experiment to those predicted by the computational model.



To define structural properties of the menisci, the lateral and medial meniscal geometries were first discretized radially resulting in 34 and 31 elements, respectively, following the method of Guess et al. [49] (Fig. 6). A linear stiffness matrix was then used to connect neighboring elements, yielding multibody representations of deformable meniscal geometries [49].

Ligament fibers were represented with straight line force elements connecting their tibial and femoral insertions. The structural properties of each ligament fiber were described using a tension-only, nonlinear force–elongation relationship (Eqs. (1a)and (1b)):

$$F(l, \dot{l}, l_0) = \frac{1}{n} \{ [f^*(l) + c_d \dot{l} B_1] B_2 + [K(l - (l_0 + \Delta_l)) + f^*(l_0 + \Delta_l) + c_d \dot{l} B_1] B_3 \}$$
(1a)

$$B_{1} = \operatorname{step}(l, 0, 0, l + 0.1, 1)$$

$$B_{2} = \operatorname{step}(l, l_{0}, 0, l_{0} + 0.1, 1) \times \operatorname{step}(l, (l_{0} + \Delta_{t}), 1, (1b))$$

$$(l_{0} + \Delta_{t}) + 0.001, 0)$$

$$B_{3} = \operatorname{step}(l, (l_{0} + \Delta_{t}), 0, (l_{0} + \Delta_{t}) + 0.001, 1)$$

where *n* is based on the number of fibers and their arrangement [16], *l* is the interinsertional distance, *l* is the first derivative of the interinsertional distance with respect to time, and  $l_0$  is the ligament slack length.  $f^*(l)$  is a cubic spline representing the ligament force–elongation response in the toe region. It was obtained by directly digitizing plots of the ligament force–elongation response from the literature [44,51–53] (GRAPHCLICK, Arizona Software, AZ). *K* represents the linear portion of the force–elongation response [44,51–54]. The transition between the toe region and linear region is defined by  $\Delta_t$  (Fig. 7). Each force element also included a parallel damping term ( $c_d = 1.5$  Ns/mm) based on the stress relaxation



Fig. 6 Overview of the multibody model including bony geometries, articular cartilage, discretized menisci, and ligament fibers

response of ligaments [55]. The step functions  $B_1$ ,  $B_2$ , and  $B_3$  are cubic polynomials that allow continuous and smooth generation of tensile forces as a ligament fiber becomes taut. The locationdependent structural properties of the AM, AL, and PL groups of the ACL were defined based on the work of Butler et al. [44]. The structural properties of the ALL were assumed to be half of the LCL based on the observation that the ALL is thinner and less stout than the LCL. The structural properties of the posterior capsule were described using a cubic spline fit to the properties of the sMCL [51], since both have a stout appearance based on visual inspection. The horn attachments of the menisci were modeled with a linear tension-only force-elongation response and a stiffness of 180 N/mm [54]. Tibiomeniscal coronary ligaments were also modeled as tension-only linear springs with a stiffness about half that of the sMCL. The transverse intermeniscal ligament was not modeled due to its insubstantial appearance during dissection of the cadaver knee. The structural properties of all the ligament fibers are summarized in Appendix B.

A generalized reduced gradient optimization algorithm was utilized to determine the slack lengths  $(l_0)$  of the ligament fibers [56]. This optimization included the 29 fibers comprising nine ligaments that were observed to be taut at full extension or that carried force at full extension in our physical experiment. The goal of the optimization was to identify  $l_0$  as a percentage of the fiber length at full extension  $(l_e)$  in the groups of fibers comprising each ligament. The objective function described the differences between the resultant ligament forces predicted by the model  $(F_i^m)$ and the experimentally measured ligament forces at full extension  $(F_i^e)$  (Eq. (2a)). The predicted ligament force was the resultant vectoral magnitude of force in the fibers comprising each ligament. Altogether, lo was optimized for 29 fibers across nine ligaments in this underdetermined system of equations (Eq. (2a)). The initial value of  $l_0$  was defined to be the fiber length at full extension, and  $l_0$  was allowed to vary  $\pm 10\%$  from the initial value (Eq. (2b))

$$\min\sum_{i=1}^{9} \left( \left| \sum_{j=1}^{a_i} \mathbf{F}_{i,j}^m(l, \dot{l}, l_0) \right| - F_i^e \right)^4 \tag{2a}$$

a is the number of fibers comprising each of the nine ligaments included in the optimization

 $F_i^m = \{\text{ACL, sMCL, LCL, FFL, OPL, POL, MPC, LPC, PCL_{PM}\}}$   $F_i^e = \{37, 4, 20, 1, 10, 18, 1, 4, 10\} \text{ N}$   $a_i = \{6, 6, 1, 1, 2, 3, 3, 3, 4\} \text{ fibers}$  $l_0 = l_e(100 - x)\% - 10 \le x \le +10$ 

(2*b*)



Fig. 7 Representative force–elongation response for a ligament fiber consisting of the slack length ( $l_0$ ), the toe region  $f^*$  (l), linear region (K), and a term ( $\Delta_t$ ) that identifies the transition between the toe and linear regions

The optimization was performed with the knee at full extension while permitting the tibia to move in the proximal–distal direction under 10 N of compression. This resolved penetration between the cartilage and meniscal surfaces, which was  $\leq 0.7$  mm due to uncertainty in the segmentation and registration of the CT-derived morphologies. The remaining degrees-of-freedom were held constant matching those of the physical experiment.

The groups of proximal and distal fibers comprising the sMCL were each assigned to carry the experimentally measured force in the entire sMCL since they were in series. The PM fibers of the PCL were included in the optimization to achieve their experimentally measured force at full extension because these fibers were observed during dissection to be taut at full extension.

Ligaments that were observed to be slack or that did not carry force at full extension in our physical experiment were not included in the optimization. The AL fibers of the PCL were observed to be slack at full extension; therefore, their slack lengths were defined based on their computed longest length obtained from the experimentally measured flexion path. The ALL was also observed to be slack at full extension; therefore, the slack length of the ALL fiber was increased by 10% of its length at full extension. The slack lengths of all the fibers of the coronary ligaments were assumed to be their lengths at full extension. The fibers of the MPC and LPC became slack with flexion in the experiment; thus, these groups were deactivated at flexion angles >30 deg.

Wrapping of the sMCL was modeled by connecting its proximal and distal fiber groups with 1 mm diameter spheres located  $\sim$ 10 mm distal to the joint line (Fig. 8). Each sphere was constrained tangent to the proximal surface of the tibia via a planar joint and constrained within this plane using a linear spring. This spring was assigned a stiffness ten times less than that of the sMCL based on the compliant connection that we observed between the sMCL and the proximal tibia during dissection.

Simulation of Passive Knee Flexion. The boundary conditions defined in the computational model of passive flexion matched those in the physical experiment. The femur was fixed in all directions except for rotation about the transepicondylar axis. The tibia was fixed in flexion, but free to translate and rotate in all other directions. Passive flexion was modeled by rotating the femur about the transepicondylar axis from full extension to 130 deg at a rate of 1.35 deg/s while applying 10 N of compression. The femur was rotated at this angular velocity to model the slow rate of loading in the robot experiment. The tibial and femoral coordinate systems and the description of knee kinematics were the same as in the physical experiment.

*Solver Parameters.* The equations of motion were generated and solved using ADAMS. The simulation process required setting up run time and solver parameters (GSTIFF integrator) [57] including an integrator error of 0.001, maximum number of iterations of ten, and initial simulation step size of 0.05 s. The simulation required 85 min to complete using a desktop computer (3 GHz Intel Xeon E5-1607 Processor) with 24 GB of RAM.

Model Evaluation. The ligament forces and tibiofemoral kinematics predicted in our computational model were compared to their corresponding measurements from the physical experiment. Force borne by knee ligaments (ACL, PCL, LCL, sMCL, and POL) was measured. The kinematics outcomes were: (1) transverse plane motion including internal-external rotation; (2) sagittal plane motions including posterior-anterior and proximal-distal translations; and (3) frontal plane motions including medial-lateral translation and varus-valgus rotation. The model outputs were discretized into 1 deg increments to compare with the 1 deg increments of data obtained in the physical experiment. To address our hypotheses, we calculated the root mean square (RMS) difference between model and experiment of each outcome across the entire flexion path. We also compared the maximum forces in the passive stabilizers across the entire flexion path as predicted by the model and measured in the physical experiment.



Fig. 8 The three proximal and three distal fibers of the sMCL were connected in series with 1 mm diameter spheres to simulate wrapping

#### Results

Following optimization, predicted ligament forces were within 0.8 N of those measured in the physical experiment at full extension. Slack lengths determined by the optimization routine ranged from 0.0% (sMCL) to 5.1% (POL) of ligament fiber lengths at full extension (Table 1).

It was hypothesized that our multibody knee model would capture low ligament forces during passive flexion from full extension through deep flexion. None of the predicted ligament forces differed from their respective experimentally measured magnitudes across the entire range of passive flexion (0–130 deg) by more than 5.7 N RMS (Table 2). Maximum force in the ACL occurred at full extension reaching 19 N and 37 N in the model and experiment, respectively. The force rapidly dropped with knee flexion in both the model and the experiment from full extension to 20 deg flexion (Fig. 9(*a*)). In the model, the force borne by the ACL achieved a constant level of 2 N from 20 to 50 deg flexion and then decreased to zero for the remainder of the flexion path. In the experiment, ACL force maintained a relatively constant tension of 5 N from 20 deg through deep flexion.

Force in the PCL dropped rapidly from full extension to 10 deg flexion in both the model and the experiment (Fig. 9(b)). The predicted PCL force then gradually increased to a maximum of 9 N at 90 deg flexion. Similarly, the experimentally measured force in the PCL gradually increased to a maximum of 7 N at 93 deg flexion.

Forces borne by the sMCL were no more than 8 N and 6 N in the model and the experiment, respectively (Fig. 9(c)). LCL force was maximum at full extension in both the model (17 N) and the experiment (20 N) (Fig. 9(d)). Force in the LCL rapidly decreased in both the model and the experiment as the knee flexed beyond full extension reaching a minimum at 20 deg and 10 deg flexion, respectively. Similarly, force in the POL was maximum at full extension in both the model (16 N) and the experiment (18 N) and rapidly decreased reaching a minimum at 20 deg and 10 deg flexion, respectively (Fig. 9(e)).

It was hypothesized that our multibody knee model would capture coupled internal rotation and anterior translation of the tibia through passive flexion from full extension through deep flexion. The predicted tibial internal rotation differed from the experimentally measured data by 1.6 deg RMS across the entire range of flexion (Table 3; Fig. 10(a)). In the sagittal plane, the tibia

Table 1 Scale factor in percent relating the fiber length at full extension ( $I_e$ ) to the slack length ( $I_o$ )

	sMCL	LCL	ACL	$\text{PCL}_{\text{PM}}$	MPC	LPC	POL	OPL	FFL
$(1 - {l_0}/{l_e})\%$	0.0	2.6	2.9	2.5	0.5	1.1	5.1	2.7	0.6

Note: Superficial medial collateral ligament (sMCL), lateral collateral ligament (LCL), anterior cruciate ligament (ACL), posteromedial fiber of the posterior cruciate ligament (PCL<sub>PM</sub>), medial posterior capsule (MPC), lateral posterior capsule (LPC), posterior oblique ligament (POL), oblique popliteal ligament (OPL), and fabellofibular ligament (FFL).

Table 2 RMS difference between experimentally measured and predicted ligament forces during passive flexion from 0 to 130 deg

RMS (N)								
ACL	PCL	sMCL	LCL	POL				
5.5	2.7	2.2	5.7	3.3				

Note: Anterior cruciate ligament (ACL), posterior cruciate ligament (PCL), superficial medial collateral ligament (sMCL), lateral collateral ligament (LCL), and posterior oblique ligament (POL).

translated anteriorly a total of 22.9 mm and 23.7 mm in the model and the experiment, respectively (Fig. 10(*b*)), with an RMS difference of 0.4 mm across the entire range of passive flexion. The predicted tibial distal translation differed from the experimental measurement by 0.7 mm RMS across the entire range of flexion (Fig. 10(*c*)). In the frontal plane, the model was offset more in varus compared to the experiment with an RMS difference of 1.8 deg and a maximum difference of 3.0 deg at 130 deg flexion (Fig. 10(*d*)). The tibia translated 2.3 mm medially in the model from 0 to 30 deg flexion, which differed from the experimental measurements by 0.5 mm. The model predicted increasing medial tibial translation of 2.8 mm from 30 to 130 deg flexion (Fig. 10(*e*)); however, the tibia translated laterally by 1.1 mm from 30 to 130 deg flexion in the experiment.

## Discussion

A multibody computational model of the native knee was developed that included a detailed representation of the soft tissue envelope comprised of 42 ligament fibers. This included six and seven fiber representations of the ACL and PCL, respectively, in concordance with previous recommendations for the minimum number of fibers needed to capture their direction-dependent tensile behavior [23,25]. Slack length of the ligament fibers was determined using experimentally measured ligament forces at full extension and an optimization routine. The formulations for slack length and architecture of the ligament fibers produced ligament force patterns over a large range of passive flexion from full extension to deep flexion (130 deg) that agreed with subjectspecific experimental measurements (Fig. 9; Table 2). These results supported our first hypothesis. The model also demonstrated important features of passive knee flexion including coupled internal rotation and coupled anterior translation from 0 to 130 deg flexion (Figs. 10(a) and 10(b)), thus supporting our second hypothesis.

A novel feature of the model is that the predictions of ligament forces and kinematics through 130 deg of passive flexion were made given only the ligament forces and the position and orientation of the knee at full extension. Moreover, the prediction of coupled internal rotation with flexion agrees with previous studies that described flexion–extension using the transepicondylar axis [3,4].

The focus of this study was passive knee flexion through a large funtionally-important range of motion since it is a common periand intra-operative clinical examination. This range of flexion introduces large changes in the relative orientation of the tibial and femoral insertions of each ligament including the cruciates [58]. When the ACL was represented as two-fibers, predicted force patterns in this ligament could not capture subject-specific experimental measurements over this large flexion range [12]. In contrast, our method for defining slack lengths and architecture of the fibers comprising the cruciates and collaterals yielded ligament force patterns that agreed well with subject-specific in situ force measurements (Table 2). Furthermore, the fibers representing the ACL captured nonuniform force patterns through flexion as previously described by Markolf et al. [59] (see Appendix C). Overall, this agreement provides a baseline to assess the response



Fig. 9 Ligament force predicted by the model (solid line) and measured in the physical experiment (dashed line) during passive flexion from 0 to 130 deg: (*a*) ACL, (*b*) PCL, (*c*) sMCL, (*d*) LCL, and (*e*) POL



Fig. 10 Tibial kinematics with respect to the femur predicted by the model (solid line) and measured in the physical experiment (dashed line) during passive flexion from 0 to 130 deg. A positive direction indicates: (*a*) internal rotation, (*b*) anterior translation, (*c*) distal translation, (*d*) varus rotation, and (*e*) lateral translation.

Table 3RMS difference between the experimentally measuredand predicted kinematics during passive flexion from 0 to130 deg

RMS	translation (m	RMS rotation (deg)		
Anterior	Distal	Lateral	Internal	Varus
0.4	0.7	2.1	1.6	1.8

of the knee model to additional diverse loading conditions including those characteristics of functional activities and laxity testing.

The forces that were measured in the PCL and ACL in our cadaver experiment corroborated previous in situ measurements during passive flexion. In a similar robotic experiment, Hoher et al. [19] measured maximum in situ PCL forces of  $15 \pm 3$  N in nine cadaver knees at 90 deg of passive flexion. These data agree with the magnitude and angle at which force was highest in our in situ measurement (9 N at 90 deg). In a study of 17 cadaver knees, Markolf et al. [20] reported average ACL forces of  $42 \pm 10$  N at full extension. These data agree with the in situ ACL force measurement of 37 N at full extension in our cadaver.

Novel strategies to estimate slack length of ligament fibers and to describe cruciate fiber architecture were developed that yielded low ligament forces through passive flexion. In a previous study by Bloemker et al., slack lengths were estimated by measuring the maximum straight line distance between ligament insertion sites, and a correction percentage was subsequently applied [8]. This resulted in large reductions (15-25%) in the maximum straight line distance of the ligament fibers. In contrast, the largest reduction in straight line distance at full extension in the present study was 5.1% (Table 1). Ligament forces were not reported in this previous study, but we speculate that they were higher than our in situ measurements given the larger reductions in fiber length [8]. In a previous study by Moglo and Shirazi-Adl, ligament slack lengths were adjusted at full extension to achieve a pretension in the collateral ligaments and ACL [9]. This technique resulted in forces carried by the cruciates and the LCL exceeding 30 N from 60 to 90 deg of passive flexion, which was at least three times greater than the corresponding in situ ligament forces that we measured (Fig. 9).

The toe region of the force–elongation response of each ligament fiber was defined on a ligament-by-ligament basis. However, the same term (usually 3% strain) is often applied to all ligament fibers [8,10,11,16,21,27]. Using our approach, the toe region varied from 1.2% to 3.7% strain across ligament fibers (see Appendix B). Thus, using a generic term for the toe region instead of a ligament-specific value likely impacts model predictions of kinematics and soft tissue forces.

The model has limitations. Our technique for determining slack lengths of the ligament fibers using optimization does not account for ligaments that are unloaded in full extension; however, this approach could be extended to flexion angles where they do carry force. Moreover, model predictions might be further improved by optimizing the individual force components of each ligament instead of only the force magnitude.

Kinematics predictions were most different from the experiment in the frontal plane. Since the ACL resists medial translation and valgus angulation [33,60], adding an additional pretension to the AL fibers of the ACL, which appear to be taut through passive flexion [58], may resolve this discrepancy. Including wrapping for the POL and incorporating multiple force elements representing the AL and PL bundles of the ACL could also prevent medial tibial translation. The ACL and PCL fibers did not intersect in deeper flexion in our model. Therefore, wrapping of the cruciate fibers in deeper flexion was not included. Since the cruciates bear little force in deeper flexion [20], wrapping of the cruciates probably does not have a major role in passive flexion at deeper angles.

Another limitation of our study was that we used population mean structural properties to describe the force–elongation response of the ligaments including the toe and subsequent linear regions. Including subject-specific ligament properties might improve agreement between model and experiment. However, the focus of this work was to develop a formulation for slack length because ligament forces and knee kinematics were previously reported to be highly sensitive to this parameter [8,9,13]. Furthermore, force in the individual fibers was not presented since this was not measured experimentally. Uncertainty analysis could be used to further explore the sensitivity of ligament forces to fiber slack length and fiber architecture.

A simplified rigid body contact formulation was utilized to describe contact between opposing articular surfaces; however,

Blankevoort et al. reported that deformable contact resulted in minimal differences in the motion patterns compared to rigid body contact in response to low levels of applied load [7]. Neither the patellofemoral joint nor surrounding muscle-tendon units were included in the model since their role is minimized during passive flexion. The initial focus of the modeling effort was passive knee flexion because it is a common clinical assessment performed by the surgeon in the examination and operating rooms.

Magnetic resonance imaging (MRI) could also be used to identify the attachments and paths of the ligaments; therefore, MRI is important for future in vivo modeling. However, in this cadaver study, CT assessment of bony prominences and depressions, dissection of the knee, and the anatomical knowledge of our clinical coauthors were adequate for defining the ligament fibers.

There are uncertainties in both the physical experiment (e.g., robot resolution, compliance, convergence tolerance, measured ligament forces, and image segmentation) and model parameters (e.g., stiffnesses, multifiber representations and attachment sites of the ligaments, and meniscal properties). Quantifying such areas of uncertainty will help identify critical factors driving knee function and will be important to assess the ability of the model to capture subject-specific differences in model predictions [61]. Since the data from our physical experiment agree well with previous measurements of knee kinematics and cruciate forces, they are adequate as an initial evaluation of our modeling approach. Future probabilistic analysis of unknown or uncertain model parameters should improve our understanding of the interplay between passive structures, such as ligaments and articular geometries, and knee kinematics.

In summary, a description of the multifiber architecture of the cruciates and a novel method to identify the slack length of ligament fibers in a computational knee model were presented. This model formulation predicted experimental findings of low ligament forces, coupled anterior translation, and coupled internal rotation through a large range of passive flexion. The model could ultimately be valuable in planning surgeries that rely on restoring the interplay between passive ligamentous and articular stabilizers, kinematics, and ligament forces. Such surgeries include ligament reconstructions, and bicruciate retaining, unicondylar, and total knee replacements.

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#### Nomenclature

- a = number of fibers for each ligament
- ACL = anterior cruciate ligament
- AL = anterolateral
- ALL = anterolateral ligament
- AM = anteromedial
- B = step function
- $c_d =$  parallel damping term
- $f^*(l)$  = cubic spline representing the ligament
- force–elongation response in the toe region  $F_i^e$  = experimentally measured ligament force at full
- extension
- $F_i^m$  = ligament force predicted by the model
- FFL = fabellofibular ligament
  - i = number of ligament included in the optimization routine
  - $\dot{l}$  = first derivative of the interinsertional distance with respect to time
  - K = linear portion of the force–elongation response
  - l = interinsertional distance for each fiber

- $l_e$  = fiber length at full extension
- $l_0 =$  ligament fiber slack length
- LCL = lateral collateral ligament
- LM = lateral coronary ligament LPC = lateral posterior capsule
- $LM_{horn} = lateral meniscus horn attachment$
- MM = medial coronary ligament
  - MPC = medial posterior capsule
- $MM_{horn}$  = medial meniscus horn attachment n = variable based on the number of fibers and their arrangement
  - OPL = oblique popliteal ligament
  - PCL = posterior cruciate ligament
  - PL = posterolateral
  - PM = posteromedial
  - POL = posterior oblique ligament
- RMS = root mean square
- sMCL = superficial medial collateral ligament
- sMCL<sub>sphare2Tib</sub> = superficial medial collateral ligament connections to the proximal tibia
  - x = variable that allowed to vary in a range of  $\pm 10$
  - $\Delta_t$  = transition between the toe region and linear
  - region

## Appendix A

All the knee geometries and ligament insertions were transformed from the CT coordinate system to the femoral coordinate system  $({_{CT_f}}^F T)$  defined in our robotic experiment using a series of rigid body matrix multiplications (Fig. 11(*a*); Eq. (A1); Table 4). Then, the relationship between the tibial coordinate system with respect to the femoral coordinate system





Fig. 11 (a) Schematic describing the transformations used to register the CT-derived geometries to the anatomical coordinate system of the physical experiment. This included the reference frames for the CT scanner (CT), the digitizer (D), and the L-frames (L) identified both in CT and via the digitizer. The anatomical coordinates systems for the tibia (T) and femur (F) were based on the digitization points (P1-P5). All the symbols are summarized in Appendix A, Table 4. (b) Image of the validation jig used to quantify the accuracy of the method employed to register the CT-derived geometries to the anatomical coordinate system.

Table 4 Symbols and notations

Coordinate s	ystems
D	Digitizer
$CT_f$	Computed tomography (femur)
$CT_t$	Computed tomography (tibia)
F	Femur
Т	Tibia
$L_{D_f}$	Femoral L-frame identified via digitizer
$L_{D_{\ell}}$	Tibial L-frame identified via digitizer
$L_{C_f}$	Femoral L-frame identified via computed tomography
$L_{C_t}$	Tibial L-frame identified via computed tomography
Anatomical	landmarks
P. P. P. P	and P-Five anatomical landmarks

was determined  $_{T}^{F}T$  (Eq. (A2)). Subsequently, the tibia geometries identified in the CT coordinate system were transformed to the femoral coordinate system,  $_{CT_{f}}^{F}T$  (Eq. (A3)) and combined with Eq. (A2) to describe the tibia relative to the femur.

The accuracy of the method was quantified using a customfabricated validation jig, which modeled all the coordinate systems used in the registration procedure (Fig. 11(*b*)). The validation jig was 18 cm in length and 36 cm in width. It consisted of Lframes representing those attached to the tibia and the femur, and five points representing the anatomical landmarks that defined the anatomical coordinate systems of the tibia and femur. The validation jig was fabricated using a computer-controlled milling machine with accuracy of  $\pm 7.62 \,\mu\text{m}$  ( $\pm 0.0003$  in.) and drilling accuracy of  $\pm 0.127 \,\text{mm}$  ( $\pm 0.005$  in.). Accuracy was represented in the anatomical coordinate system used in this study. The registration technique had a positional accuracy of 0.15 mm, 0.60 mm, and 0.27 mm in the *x* (proximal–distal), *y* (medial– lateral), and *z* directions (anterior–posterior), respectively, and 0.17 deg, 0.06 deg, and 0.09 deg about the *x* (internal–external rotation), *y* (flexion–extension), and *z* (varus–valgus) axes, respectively,

$${}_{CT_f}{}^FT = \begin{bmatrix} {}_{D}T \end{bmatrix}^{-1} \times {}_{L_{Df}}{}^TT \times {}_{L_{Cf}}{}^{L_{Df}}T \times \begin{bmatrix} {}_{CT_f}T \\ {}_{L_{Cf}}T \end{bmatrix}^{-1}$$
(A1)

$${}_{T}^{F}T = [{}_{F}^{D}T]^{-1} \times {}_{T}^{D}T$$
(A2)

$${}_{CT_{t}}{}^{F}T = {}_{T}^{F}T \times \left[ {}_{T}^{D}T \right]^{-1} \times {}_{L_{D_{t}}}{}^{D}T \times {}_{L_{C_{t}}}{}^{L_{D_{t}}}T \times \left[ {}_{L_{C_{t}}}{}^{CT_{t}}T \right]^{-1}$$
(A3)

#### Appendix B

Ligament properties (Tables 5 and 6):  $f^*(l)$  is a cubic spline describing the toe region, *K* is a linear stiffness,  $\Delta_t$  is a term that identifies the transition between the toe and linear stiffness regions,  $l_e$  is the ligament fiber length at full extension in the model, *n* is the number of fibers and their arrangement, and  $B_2$ , and  $B_3$  are the step functions.

Abbreviation for ligament fiber names: anterior cruciate ligament–ACL (seven fibers), posterior cruciate ligament–PCL (six fibers), medial- and lateral-posterior capsule–MPC and LPC (three fibers each), oblique popliteal ligament–OPL (two fibers), fabellofibular ligament–FFL (one fiber), lateral collateral ligament–LCL (one fiber), anterolateral ligament–ALL (one

Table 5 Structural properties of the fibers of each knee ligament used in the computational model

Ligament fibers	Ligament fiber names	$f^*(l)$ spline	$l_e$ (mm)	$\frac{l_0}{l_e}$ (%)	$\Delta_t (mm)$	K (N/mm)	n
1	ACL <sub>1</sub>	ACLAM	43.79	97.1	1.516	19.09	2
2	ACL <sub>3</sub>	ACLAM	36.54	97.1	1.516	19.09	2
3	ACL <sub>2</sub>	ACLAL	42.05	97.1	2.012	25.4	1
4	$ACL_4$	ACLPL	31.26	97.1	0.757	28.78	3
5	ACL <sub>5</sub>	ACLPL	32.39	97.1	0.757	28.78	3
6	ACL	ACLPL	28.94	97.1	0.757	28.78	3
7	PCL <sub>1</sub>	PCL <sub>PM</sub>	41.66	97.5	2.073	57	4
8	PCL <sub>2</sub>	PCL <sub>PM</sub>	40.44	97.5	2.073	57	4
9	PCL <sub>3</sub>	PCL <sub>PM</sub>	39.71	97.5	2.073	57	4
10	$PCL_4$	PCL <sub>PM</sub>	40.38	97.5	2.073	57	4
11	PCL <sub>5</sub>	PCLAL	35.75	110	3.011	120	3
12	PCL <sub>6</sub>	PCLAL	36.51	110	3.011	120	3
13	$PCL_7$	PCLAL	37.17	110	3.011	120	3
14 <sup>a</sup>	MPC <sub>1</sub>	sMCL	26.73	99.5		_	3
15 <sup>a</sup>	MPC <sub>2</sub>	sMCL	26.10	99.5		_	3
16 <sup>a</sup>	MPC <sub>3</sub>	sMCL	26.71	99.5		_	3
17 <sup>a</sup>	LPC <sub>1</sub>	sMCL	29.24	98.9		_	1
18 <sup>a</sup>	$LPC_2$	sMCL	31.30	98.9		_	1
19 <sup>a</sup>	$LPC_3$	sMCL	31.28	97.3	_	_	1
20 <sup>a</sup>	OPL <sub>1</sub>	POL	45.64	97.3		_	1
21 <sup>a</sup>	OPL <sub>2</sub>	POL	62.76	97.3		_	1
22 <sup>a</sup>	FFL	POL	56.89	99.4	_	_	1
23	LCL	LCL	58.64	97.4	1.505	59	1
24	ALL	LCL	47.55	110	1.505	30	1
25	$POL_1$	POL	42.03	94.9	3.021	56	3
26	POL <sub>2</sub>	POL	43.00	94.9	3.021	56	3
27	POL	POL	46.15	94.9	3.021	56	3
28	sMCL <sub>1</sub>	sMCL	39.59	100	2.517	80	2/3
29	sMCL <sub>2</sub>	sMCL	39.48	100	2.517	80	2/3
30	sMCL <sub>3</sub>	sMCL	39.45	100	2.517	80	2/3
31	sMCL <sub>4</sub>	sMCL	47.77	97.5	2.517	80	2/3
32	sMCL <sub>5</sub>	sMCL	47.76	97.5	2.517	80	2/3
33	sMCL <sub>6</sub>	sMCL	47.65	97.5	2.517	80	2/3
34 <sup>b</sup>	sMCL <sub>Sphere2Tib1</sub>		0.0			5	1
35 <sup>b</sup>	sMCL <sub>Sphere2Tib2</sub>		0.0			5	1
36 <sup>b</sup>	sMCL <sub>Sphere2Tib3</sub>	—	0.0	—	_	5	1

$${}^{b}f^{*}(l) = 0, \quad B_{2} = 0, \quad B_{3} = \text{step}(l, l_{0}, 0, l_{0} + 0.1, 1)$$

Table 6 Structural properties of the coronary ligaments and horn attachments of the medial and lateral menisci

Ligament fibers	Ligament fiber names	$f^*(l)$ spline	$l_e ({ m mm})$	$rac{l_0}{l_e}$ (%)	$\Delta_t (mm)$	K (N/mm)	n
1 <sup>b</sup>	LM <sub>Horn1</sub>	_	0.0	_		180	1
2 <sup>b</sup>	LM <sub>Horn1</sub>		0.0		_	180	1
3 <sup>b</sup>	MM <sub>Horn1</sub>		0.0		_	180	1
4 <sup>b</sup>	MM <sub>Horn2</sub>		0.0		_	180	1
5 <sup>b</sup>	$LM_1$	_	29.65	100	_	36	1
6 <sup>b</sup>	$MM_1$		7.60	100	_	36	1
7 <sup>b</sup>	$MM_2$		4.40	100	_	36	1
8 <sup>b</sup>	MM <sub>3</sub>		7.07	100	_	36	1
9 <sup>b</sup>	$MM_4$		7.04	100	_	36	1
10 <sup>b</sup>	MM <sub>5</sub>		5.07	100	_	36	1
11 <sup>b</sup>	MM <sub>6</sub>		6.54	100	_	36	1
12 <sup>b</sup>	$MM_7$		6.52	100		36	1

$${}^{a}B_{3} = 0.$$
  
 ${}^{b}f^{*}(l) = 0, \quad B_{2} = 0, \quad B_{3} = \operatorname{step}(l, l_{0}, 0, l_{0} + 0.1, 1).$ 

fiber), posterior oblique ligament–POL (three fibers), superficial medial collateral ligament–sMCL (1:3 proximal fibers and 4:6 distal fibers), superficial medial collateral ligament connections to the proximal tibia–sMCL<sub>sphare2Tib</sub> (three fibers), lateral and medial meniscus horn attachments–LM<sub>horn</sub> and MM<sub>horn</sub> (two fibers each), and lateral and medial coronary ligaments–LM (one fiber) and MM (seven fibers).

#### Appendix C

Predicted force in the individual fibers of the ACL throughout the flexion arc (Fig. 12).



Fig. 12 Predicted force in the individual fibers of the ACL throughout the flexion arc (0-130 deg): (a) AM (two fibers) and AL (one fiber); (b) PL (three fibers)

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