

Knee Model Benchmarking Specification – Denver Knee OKS03

Site: University of Denver

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1. Summary of Model Benchmarking Data

1.1 Overview

This section provides details on inputs for Phase 3: Model Benchmarking. Inputs include experimental joint laxity data for Benchmarking, as well as the deliverables obtained from Phase 1: Model Development, and Phase 2: Model Calibration.

The Model Development (Phase 1) deliverables package can be found in the following location:
<https://simtk.org/svn/kneehub/ModelDevelopment/Outcomes/>

The Model Calibration (Phase 2) deliverables package can be found in the following location:
<https://simtk.org/svn/kneehub/ModelCalibration/Outcomes/>

The Model Benchmark (Phase 3) standard calibration and benchmark cases are located here:
https://simtk.org/frs/?group_id=1061

1.2 Earmarked Experimental Data for Model Calibration

Benchmarking data consists of two cases: Benchmark Calibration and Benchmark Use Case

1.2.1 Earmarked Benchmark Standard Calibration

One file is provided in *data-MB-OKS03.zip* which includes a spreadsheet of tibiofemoral kinematics as defined by Grood and Suntay [1], loadcell data transformed to the joint coordinate system defined for kinematics, and probed point data. The experimental activities include: “Passive Flexion”, “AP”, “EI”, and “VV” with “AP” referring to anterior-posterior, “EI” referring to external-internal and “VV” referring to varus-valgus activities. A text file “DESCRIPTION” is included that describes processing of the data to achieve the standard calibration targets.

1.2.2 Earmarked Benchmark Use Case – Combined Loading

Files are provided in *data-MB-OKS03.zip* which includes spreadsheets of tibiofemoral kinematics as defined by Grood and Sunday [1], as well as loadcell data transformed to the joint coordinate system defined for kinematics. The experimental activities include: “Passive Flexion”, “AP”, “EI”, and “VV”. A text file “DESCRIPTION” is included that describes processing of the data to achieve the benchmark targets.

2. Preparation of Laxity Calibration Data

2.1 Objective

The earmarked data from OKS03 will be prepared into smaller data subsets, which will be used for calibrating ligament response. The data will be processed in a similar format and compared to the calibration data from the Model Calibration (Phase 2) process.

Primary Tools

- MATLAB (2016a), MathWorks (Natick, MA)

Input(s)

- Recalibration Data for OKS03: Kinematic and loadcell data from 4 laxity experiments (*.csv)

Output

- Corrected laxity data (.xlsx)
- Processing script "ProcessOKSLaxityData.m"

2.2 Prepare Calibration Data from Standardized Set

A custom MATLAB script was written to read in the CSV files and export files in a format consistent with DU's knee model conventions and the DU02 calibration data. The data provided for OKS03 includes laxity application at discrete angles of knee flexion: 0°, 30°, 60°, 90°. The loads are applied for a single cycle of minimum and maximum application for each degree of freedom (DOF).

- Use TDMSRead toolbox to parse the files for AP, VV, and IE laxity assessments in addition to the passive knee flexion.
- The sign convention of kinematics DOFs IE, ML, and AP DOFs were negated to develop kinematic consistency between the OpenKnee data convention and the DU knee model convention (+flexion, +valgus, +external tibia, +lateral tibia, +anterior tibia, +superior tibia).
- The sign convention of kinetic DOFs FE, IE, ML, SI were negated to develop kinetic consistency between the OpenKnee data convention and the DU knee model *applied kinetics convention* for a left knee (+medial tib, +anterior tib, +superior tib, +flexion, +varus, +internal tibia).
- The processed data were then saved into an excel spreadsheet for each loading case: OKS03_APLaxityData.xlsx, OKS03_IELaxityData.xlsx, OKS03_VVLaxityData.xlsx, and OKS03_PassiveFlexion.xlsx.

3. Model Preparation

3.1 Objective

The assignment of the model coordinate systems will be examined based on the recalibration data and may be updated, as necessary.

Primary Tools

- MATLAB (2016a), MathWorks (Natick, MA)
- Hypermesh (v2019), Altair (Troy, MI)

Input(s)

- Model files

Output

- Model files with updated joint coordinate representation
- OKS03 registration code “OKS03_Registration.m”
- OKS03 joint coordinate system building code “BuildGS_Wrapper.m”, “Build_GS_TMAT_OKS03.m”, “Calc_GS_Axes.m”

3.2 Update/Check Joint Coordinate System and Base Pose

The location of the model joint coordinate system (JCS) will be checked against the OKS03 recalibration data probed points and offsets.

3.2.1 Registration Between Testing and Scan Spaces

The State.cfg file contains descriptions of transformations between various coordinate systems and digitized probed point data in the robotic testing environment provided by Cleveland Clinic. The Recalibration data includes probed points on bones and fiducial spheres in optotrack space. The fiducial spheres affixed to the bones will be used to develop correspondence between the optotrack space and the scan/model space in the following manner:

- Using MATLAB, load the STLs extracted from the segmented fiducial spheres in the MRI scans.
- Use a sphere fitting algorithm to define the center of these spheres in scan space.
- Import data corresponding to the digitized surface position of the fiducial spheres from the recalibration file in optotrack space.
- Use a sphere fitting algorithm to define the center of these spheres in optotrack space.
- Using the center of the three spheres in two different spaces, define a local coordinate system for each space, and then calculate a transformation matrix to take data from optotrack space to scan space (T_F_SENSOR_MRI for the femur, T_T_SENSOR_MRI for the tibia).

3.2.2 Calculation of Joint Coordinate Systems

Bony landmarks were probed as part of the experimental testing protocol described in the OpenKnee wiki (/Specifications/SpecimenPreparation/). These probed points are provided in optotrack space for each respective bone. Using the coordinate system transformations described in 3.2.1, transform landmarks into the scan/model space. The probed points were added to the GS_NODES.inp simulation input file, and rigidly attached to their respective bone. This allows the modeler to extract the probed points during any simulation and calculate kinematics directly.

The probed points were used to build local femur and tibia coordinate systems following the procedures described in the “DESCRIPTION.pdf” document provided with the recalibration data. The document details the axis creation and order of operations used to build each local

coordinate system. Finally, custom code used in Phase 1 Model Development was used to build finite element connector elements defining the axes of translation and rotation of the joint coordinate systems for the tibiofemoral (TF) and patellofemoral (PF) joints.

3.2.3 Update Base Pose Kinematics in Model Files

Using the newly defined joint coordinate system, a set of kinematics was calculated for the base pose of the model. The kinematics of the initial position were necessary to prescribe accurate model kinematics through the different model calibration activities using the absolute kinematics provided in the processed recalibration laxity files for AP, VV, IE, and passive knee flexion.

4. Calibration of Ligament Parameters to Passive Knee Flexion

4.1 Objective

Passive knee flexion provides the first step in calibration of ligament geometrical representation and reference length. Ligament lengthening patterns are well described in the literature for passive flexion, and thus this activity can be used to assess uncertainty in ligament insertion and origin location in the model, tuning of reference strain to describe the onset of force through a constrained kinematic profile, and an initial guess for the optimization of ligament parameters with laxity data described in section 5.

Primary Tools

- MATLAB (2016a), MathWorks (Natick, MA)
- ABAQUS/Explicit (2019), SIMULIA (Providence, RI)

Input(s)

- Model files
- Passive flexion kinematics
- Length/strain descriptions from the literature

Output

- Updated ligament parameters files

4.2 Prepare Simulation Inputs

4.2.1 Prepare Passive Flexion Kinematics

Open OKS03_PassiveFlexion.xlsx created in section 2.2 which includes the processed passive flexion kinematics and kinetics.

Data points will be chosen from passive flexion at 0°, 30°, 60°, and 90° assembled from the zero load laxity profiles and added as targets in the excel file. Input files with kinematic and kinetic amplitudes will be assembled for a two-step simulation comprised of a settling period before performing knee flexion. Settling will allow for the bones to come into contact and move from initial pose of the model to the initial pose of the passive flexion activity. Passive flexion input files describing 6 DOF kinematics and kinetics as a function of time will be created and prepared for simulation.

4.2.2 Prepare Model Simulation Files

Model files will be modified to include a two-step simulation procedure. The first step of the FE job will be a brief ($t=0.2s$) settling step. Contact will be represented, and the superior-inferior (SI) and varus-valgus (VV) DOF will be disregarded in the kinematic profiles from the passive knee flexion, and a very small compressive load applied to SI to allow the joint to settle into contact. This is done to ensure a better calibration of ligament parameters over the as-built contours of the model condyles. The second step of the simulation will perform a kinematically driven passive flexion using the amplitudes described in Section 4.2.1, while still allowing the VV and SI DOF to solve based on the interaction of ligament and cartilage contact.

4.3 Adjustment of Ligament Parameters

Reference strain and ligament attachment position will be calibrated by manually adjusting the ligament geometry and material parameters to best match ligament loading during passive flexion results presented in literature. The initial guess for all parameters will be taken from the results of the Model Calibration Phase (Table 1). The process will begin by changing the reference strain (ϵ_0) such that the ligament loading matches trend and magnitude of previously reported results for the ACL, PCL, LCL, and MCL [2–8] (Figure 1). The posterior joint capsule will be adjusted to carry load in full extension (0° to 5° flexion). Overall, this should be a straightforward process which will require small manual changes to the reference strain values. The remaining ligaments will be checked to prevent unrealistic contribution during passive flexion ($>50N$).

Ligament footprint regions were developed in Phase 1 Model Development to characterize uncertainty through different scan sequences (OKS03) and probed point data registration (DU02) for each knee specimen (Figure 2). The second step of passive flexion calibration will assess the ligament origin footprints and force profiles as a function of flexion angle and adjust the location of the (1) footprint centroid and (2) radius of the fibers from the centroid. For the collateral ligaments this will allow the ligament to become either more narrow or broad in the anterior-posterior direction of the knee, as well as translate anterior, posterior, superior, or inferior within the ligament insertion region. For the cruciate ligament, perturbations can affect either the entire ligament (4 fibers representing two bundles each) or individual bundles (2 fibers each) to adjust the force profiles over the flexion cycle (Figure 2). These changes will be informed by the results seen in the previous section to better correspond to relevant literature.

4.4 Updating Model and Results Reporting

Once the passive flexion calibration has been performed, updated ligament parameters files will be exported including the new ligament reference strain values. For ligaments which underwent changes to origin footprint geometry, updated `LIG_*.inp` files will also be exported. Graphical and numerical results highlighting targets as well as calibrated and uncalibrated ligament response will also be exported and delivered with mid-point model calibration results.

Table 1. Initial guess of ligament properties for Benchmark Calibration based on the results from the prior Model Calibration Phase.

Ligament/Bundle	Stiffness (k)	Reference Strain (ϵ_0)
ACLam	68.9	1.087
ACLpl	105.8	0.996
PCLpm	54.9	1.001
PCLal	35.3	0.881
LCL	148.4	0.951
MCLa	97.9	0.968
MCLm		1.041
MCLp		1.085
dMCL	40.5	1.041
PCAPm	90.0	0.900
PCAPI	90.0	0.900
POL	50.3	1.034
ALS	29.3	0.834
PFL	37.3	1.079

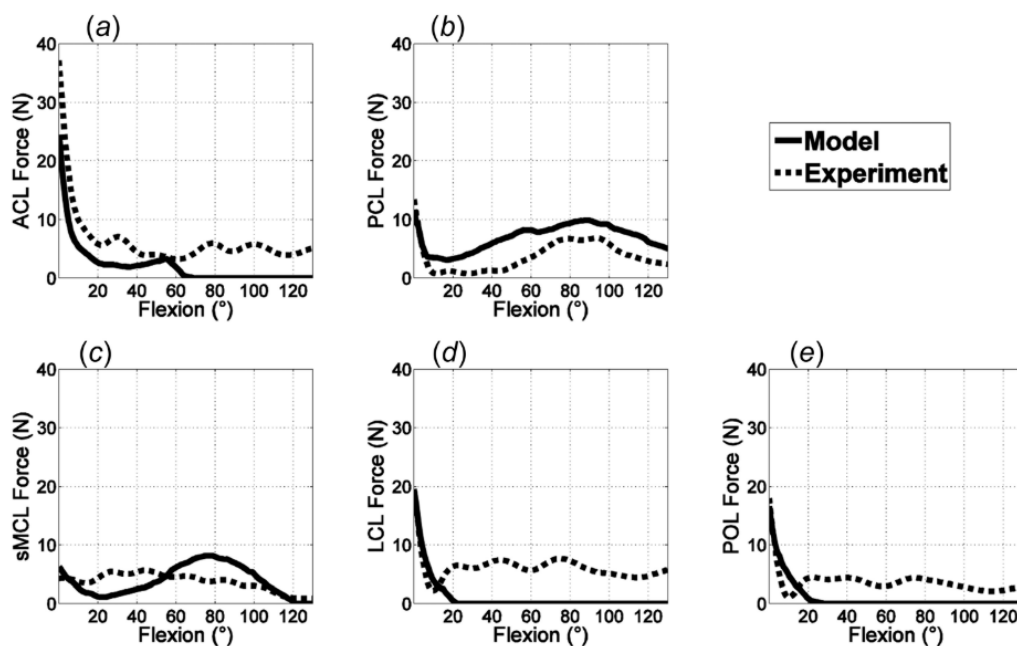


Figure 1. Reproduction of Figure 9 from Kia et al. (2016) illustrating experimental and modeling ligament force profiles during a passive flexion experiment.

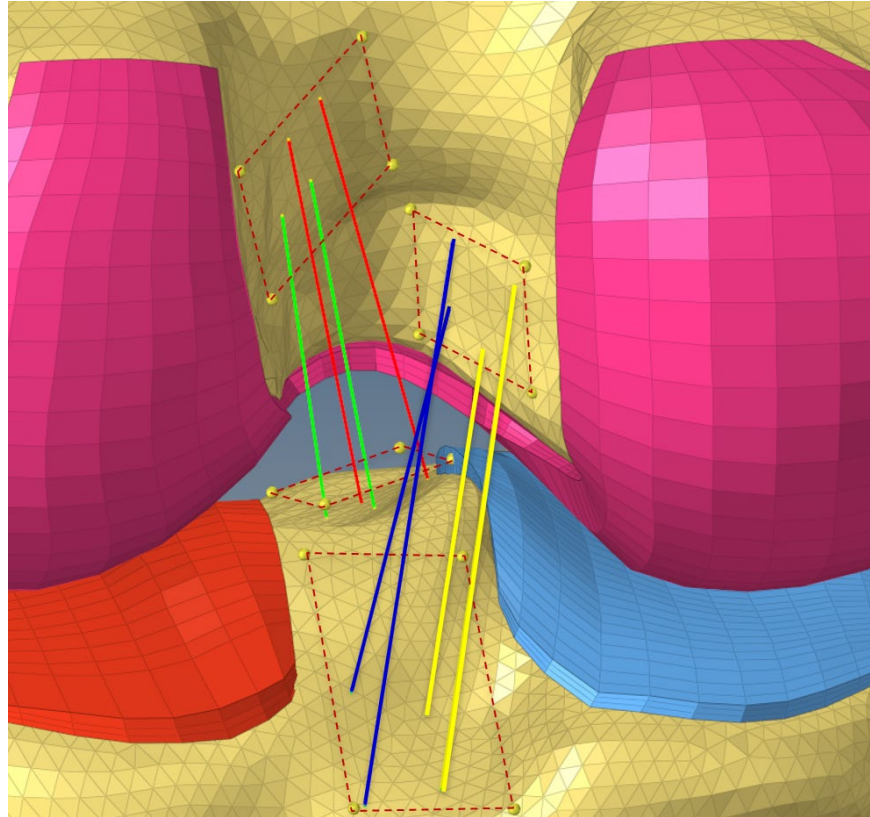


Figure 2. Representation of ligament footprint regions of the ACLam, ACLpl, PCLpm, and PCLal for use in calibration during the passive flexion simulation.

5. Calibration of Ligament Parameters to Laxity Experiments

5.1 Objective

The objective is to build an accurate representation of the kinematic envelope of the knee using laxity data in anterior-posterior, internal-external, and varus-valgus degrees of freedom. The continued calibration of ligament stiffness and reference strain while constraining the design variables within physiological bounds will provide an efficient method to accomplish this goal. Targets will be determined from the csv files within the RECALIBRATION ProcessedData folder (section 2).

Primary Tools

- ABAQUS/Explicit (2019), SIMULIA (Providence, RI)
- MATLAB (2016a), MathWorks (Natick, MA)

Input(s)

- Model files
- Laxity loads and kinematic targets

Output

- Updated ligament parameters files
- OKS03 ligament optimization code “LigCalibration_Wrapper.m” and nested functions

5.2 Prepare Simulation Inputs

5.2.1 Prepare Laxity Kinematic Targets

Preparation of experimental laxity data into useable loading profiles or targets is an important step before simulation. The laxity curves prepared in Section 2.3 represent a region of minimum (max negative) and maximum (max positive) load application, such as max posterior force to max anterior force, occurring at four distinct joint angles (0°, 30°, 60°, 90°). Input files representing these load applications will be assembled by choosing regions of max loading in various degrees of freedom. The data points used for calibration will include loads and joint kinematics recorded at 8 distinct positions (e.g. 4 flexion angles, one maximum negative load/torque, and one maximum positive load/torque) for each laxity assessment (AP, VV, and IE). In total, 24 simulations will be evaluated in parallel to assess the performance of the cost function throughout the optimization (Table 2 **TBD**).

The optimization will include an initial convergence criterion consisting of an RMSE of 2 (° or mm) for each activity. In situations where AP, IE, and VV laxity simulation errors all satisfy $RMSE < 2$, additional experimental targets may be added to further constrain the laxity response.

5.2.2 Prepare Model Simulation Files

Input files for kinematics and simulation will be prepared to match the data prepared in 5.2.1. This will be achieved using a series of one-step Abaqus simulations. The first phase of simulation will flex the knee to one of four desired flexion angles (0°, 30°, 60°, 90°) and allow for a brief period of settling. The second phase will then apply the eight different loading profiles for min and max load at each of the four flexion angles. The resulting rotation or displacement of the joint will then be compared to the expected targets obtained from the experimental data and used to calculate the cost function defined as the sum of the squared RMSE.

5.2.3 Prepare Simulation JobQueue

Running 24 simulations in parallel is likely a difficult task on most desktop workstations due to hardware constraints. To help manage the various processes a previously developed JobQueue software will be used to manage the various steps and parallelization of the process. The JobQueue API developed in MATLAB will allow for extensible parallelization depending on the number of CPU cores available during runtime. As an example, the 24 simulations required for the second step can easily be restructured as 2 sets of 12 parallel simulations, or 1 set of 24 parallel simulations. This will drive flexibility and efficiency in computation burden. Figure 3 illustrates the optimization workflow.

5.3 Perform Optimization

The optimization will begin using the ligament parameters obtained in Section 4 from the passive flexion calibration. The optimization framework is housed in MATLAB using a modified Nelder-Mead bounded downhill simplex and will take advantage of the JobQueue API described previously.

Table 2a. Target kinematics (deg, mm) and loading (N, N*mm) used for the anterior-posterior optimization simulations.

Sim #	FE	VV	IE	ML	AP	SI	Force ML	Force AP	Force SI	Torque FE	Torque VV	Torque IE
1	0											
2	30											
3	60											
4	90											
5	0											
6	30											
7	60											
8	90											

Table 2b. Target kinematics (deg, mm) and loading (N, N*mm) used for the varus-valgus optimization simulations.

Sim #	FE	VV	IE	ML	AP	SI	Force ML	Force AP	Force SI	Torque FE	Torque VV	Torque IE
1	0											
2	30											
3	60											
4	90											
5	0											
6	30											
7	60											
8	90											

Table 2c. Target kinematics (deg, mm) and loading (N, N*mm) used for the internal-external optimization simulations.

Sim #	FE	VV	IE	ML	AP	SI	Force ML	Force AP	Force SI	Torque FE	Torque VV	Torque IE
1	0											
2	30											
3	60											
4	90											
5	0											
6	30											
7	60											
8	90											

5.3.1 Optimization Design Variables

The optimization design vector will include the reference strain and stiffness of each ligament, with some ligaments further divided into functional bundles. An example of this is the separation of properties for the anterior, medial, and posterior bundles of the superficial MCL, as well as separate bundles of the PCL and ACL (Table 3). The resulting design vector contained 26 variables.

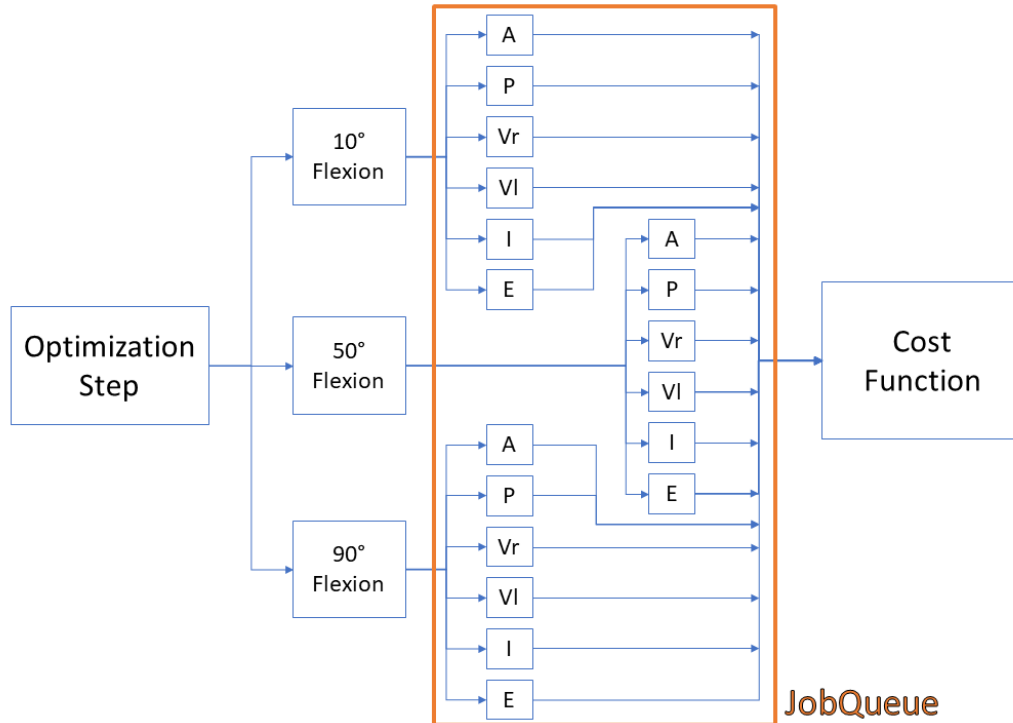


Figure 3. Visual representation of a single design vector evaluation. While the schematic shows calibration at 10°, 50°, and 90°, the calibration is performed at 0°, 30°, 60°, 90°. The simulation process involves first flexing knee to desired flexion angle, and then applying anterior (A), posterior (P), Varus (Vr), Valgus (VI), Internal (I), and External (E) loading in second step. The resultant model position will then be compared to the kinematic targets and applied as the cost function.

Upper and lower bounds for design variables have been established based on previous work and ranges reported in literature [9–13] (Table 4). Initial guesses for reference strain will come from the calibration performed on the passive flexion experiments as described in Section 4. Initial guesses for ligament stiffness will be based on previously calibrated results for the DU02 knee model [14].

The ligament parameters corresponding to the medial and lateral posterior capsule (PCAPM, PCAPL) were slackened to ensure they don't overly contribute during calibration at full extension, and their bounds clamped to prevent unnecessary computational time. In lieu of laxity calibration, the resistance in full extension will be calibrated using passive flexion data

and discussed in Section 5.3.3. The original bounds for the posterior capsule were 50-110 (N/mm) for stiffness and 0.75-1.25 for reference strain.

Table 3. Variables and structures contained in the design vector for the ligament optimization of knee laxity experiments. The anterior, medial, and posterior fibers representing the MCL have different reference strains.

Ligament/Bundle	Stiffness (k)	Reference Strain (ϵ_0)
ACLam	X	X
ACLpl	X	X
PCLpm	X	X
PCLal	X	X
LCL	X	X
MCLa	X	X
MCLm		X
MCLp		X
dMCL	X	X
PCAPm	-	-
PCAPI	-	-
POL	X	X
ALS	X	X
PFL	X	X

Table 4. Upper and lower bounds for stiffness (N/mm) and reference strain in the optimization.

Ligament /Bundle	Stiffness (k) Lower Bound	Stiffness (k) Upper Bound	Reference Strain (ϵ_0) Lower Bound	Reference Strain (ϵ_0) Upper Bound
ACLam	50	150	0.85	1.15
ACLpl	50	150	0.85	1.15
PCLpm	30	100	0.85	1.15
PCLal	30	100	0.85	1.15
LCL	60	200	0.85	1.15
MCLa	60	180	0.85	1.15
MCLm			0.85	1.15
MCLp			0.85	1.15
dMCL	50	180	0.85	1.15
PCAPm	90	90	0.90	0.90
PCAPI	90	90	0.90	0.90
POL	30	90	0.75	1.25
ALS	20	140	0.75	1.25
PFL	10	90	0.75	1.25

5.3.2 Optimization Cost Function

The optimization will utilize a cost function of the sum of the squared RMSE from each activity. An initial convergence criterion will be implemented consisting of an RMSE of 2 (° or mm) for each activity. In situations where AP, IE, and VV laxity simulation errors all satisfy $RMSE < 2$, additional experimental targets may be added to further constrain the laxity response. If the target matching RMSE's do not reach 2, optimization stopping criteria are assigned in MATLAB: function and variable tolerances are set to $1e-2$.

Given the nature of the error between the simulations and experimental targets including a combination of millimeters and degrees there will need to be a combined cost function which includes both units. This will be implemented as an unscaled combination of the RMSE (mm) from AP combined with the RMSE (deg) from the VV and IE activities. If the errors appear to be on different orders of magnitudes, scaling factors will be added to weight the combination of units.

In addition to the scaling factors for AP, VV, and IE target matching, secondary DOFs were identified for each activity that play a crucial role in ligament loading for that task. The list of cost functions components and weights utilized in the optimization is found in Table 5.

Table 5. Final cost function components and weights.

Cost Function Parameter	Weight
AP DOF (primary) during AP Laxity	1
IE DOF (secondary) during AP Laxity	0.5
IE DOF (primary) during IE Laxity	1
AP DOF (secondary) during IE Laxity	0.5
VV DOF (primary) during VV Laxity	1
IE DOF (secondary) during VV Laxity	0.5

5.3.3 Calibration of Posterior Joint Capsule During Full Extension

Upon completion of the experimental laxity calibration the posterior joint capsule was calibrated using a similar technique to that described for the DU02 knee. An extension torque of 10 Nm was applied to the model and the model was freely allowed to deform kinematically. The reference strain of both the medial and the lateral capsule were increased until the final kinematic position of the joint matched 0°. The medial and lateral capsule were adjusted such that they carried similar loads (+/- 10 N) during the extension torque application.

5.4 Calibration to Standardized Data Results TBD

5.4.1 Intermediate Outputs

Modeling and Simulation Intermediate Outputs for Model Standardized Calibration:

- Data used for Simulations – Processed data and datapoints used for Model Standard Calibration.

- Loading and Boundary Conditions – Files defining kinematics and kinetics applied during standardized calibration.
- Updated Geometry – If any, changes made to ligament insertion and origin geometry.
- Updated Coordinate Systems – If any, changes to the joint coordinate system defined in the OKS03 standardized calibration description.
- Updated Ligament Parameters – Input files describing updates made to the ligament material properties which are not considered final outputs. This can include changes made during new passive flexion simulations.
- Code – Any new versions of MATLAB code used for preprocessing of data, alignment of coordinate systems, and ligament optimization framework.

5.4.2 Endpoint Outputs

Modeling and Simulation Standardized Calibration Outputs: Taken together, the set of input files defining a finite element model of the specimen performing a passive knee flexion activity and simulations of the standardized laxity experiments.

- Documentation on Data Used – A text file describing the sections of data which were used for the various steps in standardized calibration, highlighting any data which was different from Phase 2 Model Calibration.
- Updated Model – An updated model designed for ABAQUS/Explicit simulation of passive flexion to 120° of knee flexion and laxity experiments which were used for model calibration.
- Simulation Files – Completed simulation and results file (ODB) of models described above.
- Results – Spreadsheet with ligament forces during final laxity experiments plotted against experimental data. Spreadsheet with ligament forces from passive knee flexion after model calibration phase.

6. Benchmark Case: Combined Loading

6.1 Overview

This section provides details on the outputs for Phase 3: Model Benchmarking. Outputs include the response of the calibrated knee to the OKS03 combined loading benchmark load case.

6.2 Prepare Passive Flexion Kinematics

6.2.1 Prepare Model Benchmark Data

Open OKS03_CombinedLoading.xlsx will be created as described in section 2.2 which includes the processed benchmark kinematics and kinetics.

6.2.2 Prepare Model Simulation Files

Input files for kinematics and simulation will be prepared to match the data prepared in 5.2.1. This will be achieved using a one-step Abaqus simulation. The first phase of simulation will flex the knee to one of four desired flexion angles (0°, 30°, 60°, 90°) and allow for a brief period of settling.

6.3 Deliverables from Phase 3 Model Benchmarking

6.3.1 Documentation

Finalized documentation for Model Benchmarking phase:

- Model Standardized Calibration and Benchmark Specification (Original) – The original Model Benchmark Specification as outlined in the documentation portion of Phase 3. Submitted prior to execution of model benchmarking.
- Protocol Deviation Document – Identifying changes and change locations made to the originally submitted specification and submitted with Phase 3 deliverables.
- Model Standardized Calibration and Benchmark Specification (Final, Revision A) – An updated version of the Model Benchmark Specification submitted with Phase 3 deliverables.

6.4 Model Benchmarking ACL deficient Results TBD

6.4.1 Intermediate Outputs

Modeling and Simulation Intermediate Outputs for Model Benchmarking phase:

- Data used for Simulations – Processed data and datapoints used for Model Benchmark.
- Loading and Boundary Conditions – Files defining kinematics and kinetics applied during combined loading benchmark.
- Code – Any new versions of MATLAB code used for preprocessing of data, alignment of coordinate systems, and ligament optimization framework.

6.4.2 Endpoint Outputs

Modeling and Simulation Endpoint Outputs for Model Benchmarking phase. Taken together, the set of input files defining a finite element model of the specimen performing a passive knee flexion activity and simulations of the combined loading benchmark laxity experiments.

- Updated Model – An updated model designed for ABAQUS/Explicit simulation of passive flexion to 120° of knee flexion and laxity experiments which were used for the model benchmark test case.
- Simulation Files – Completed simulation and results file (ODB) of models described above.
- Results – Spreadsheet with ligament forces during final laxity experiments plotted against experimental data. Table showing experimental and simulation key point values from benchmark data set. Spreadsheet with ligament forces from passive knee flexion of model in the combined loading condition.

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