

# Modeling and Simulation Workflow Using Open Knee(s) Data

## Model Calibration Output Descriptors

## Cleveland Clinic Approach

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# Synopsis

This document summarizes modeling and simulation outputs generated through model calibration specifications<sup>1</sup> and protocol deviations<sup>2</sup>, which were documented for the calibration of an initial working model of the knee joint based on an existing data set from the Open Knee(s) project<sup>3</sup>. The outputs and this documentation is in response to the Model Calibration phase<sup>4</sup> of the project Reproducibility in simulation-based prediction of natural knee mechanics, a study funded by the National Institute of Biomedical Imaging and Bioengineering, National Institutes of Health (Grant No. R01EB024573)<sup>5</sup>. The outputs represent those of the Cleveland Clinic team, who launched and has been maintaining the Open Knee(s)<sup>3</sup>. They correspond to a working comprehensive and extensible knee joint model incorporating anatomical and mechanical detail of its major structures.

# File Descriptors

All the file types and formats that are found in the outputs folder are described in here.

File	Description	File Format
<b>Smooth Geometry</b>	Geometric reconstruction of tissues of interest as triangulated watertight surface representations, <u>with several mesh densities for each tissue</u> . Created from raw geometry (output of <i>Model Development</i> phase <sup>6</sup> ) after applying volume-preserving smoothing procedures.	.stl <sup>7</sup>
<b>Connectivity</b>	XML based text file which specifies which geometry files will be used in the model, and the ties and contacts between tissues to be included in the model (used as input for the mesh generation, and template model generation scripts).	.xml <sup>8</sup>
<b>Mesh</b>	Finite element meshes of tissues of interest as triangulated surface (bones) or tetrahedral volume meshes (cartilage, menisci, ligaments, tendon) in binary format, <u>with several mesh densities for each tissue including converged mesh densities</u> . Created from smooth geometry with node, face, element sets to facilitate model assembly, material property definitions, and assignment of tissue interactions.	.med <sup>9</sup>
<b>Template Model (FEBio Input File)</b>	XML based text file (for finite element analysis with FEBio <sup>10</sup> ) including mesh definitions, template constitutive models (rigid – bones; deformable – other tissue), template interactions between tissue, and template loading and boundary conditions (for rigid objects); <u>including templates for mesh convergence, material property confirmation, and in situ ligament strain calibration, and post-calibration simulations of experiment conditions</u> .	.feb <sup>11</sup>
<b>Model Properties</b>	XML based text file which specifies the material properties of all tissues in the model, and the coordinates of the manually chosen anatomical landmarks (used as input for the customization script); <u>including templates for mesh convergence, material property confirmation, and in situ ligament strain calibration, and post-calibration simulations of experiment conditions</u> .	.xml <sup>8</sup>

File	Description	File Format
<b>Customized Model (FEBio Input File)</b>	XML based text file (for finite element analysis with FEBio <sup>10</sup> ) customized to include mesh definitions, tissue interactions, tissue-specific constitutive models, in situ ligament strains, representation of additional stabilizing structures, anatomical knee joint coordinate systems, specialized loading and boundary conditions to represent passive flexion, output requests relevant to knee mechanics; including numerical analysis settings; <u>including customizations for mesh convergence, material property confirmation, and in situ ligament strain calibration, and post-calibration simulations of experiment conditions.</u>	.feb <sup>11</sup>
<b>Raw Simulation Results</b>	Binary (.xplt) and text files (.log) obtained by simulation of passive flexion using <u>calibrated</u> customized model with FEBio <sup>10</sup> ; <u>in addition, results of mesh convergence, material property confirmation, and in situ ligament strain calibration, post-calibration simulations of experiment conditions.</u>	.xplt <sup>11</sup> .log <sup>11</sup>
<b>Processed Simulation Results</b>	CSV based text files storing extracted knee kinematics and kinetics during passive flexion simulations <u>using calibrated model</u> ; processed using raw simulation results and supported by graphs as binary image files; <u>in addition, processed results of mesh convergence, material property confirmation, and in situ ligament strain calibration, post-calibration simulations of experiment conditions.</u>	.csv <sup>12</sup> .png <sup>13</sup>
<b>Calibration Summary</b>	Microsoft Word (or LibreOffice Writer) based file storing images and tables summarizing decisions in Mesh Convergence and Material Properties Confirmation stages of the calibration phase.	.docx <sup>14</sup> .odt <sup>15</sup>
<b>Registration Results</b>	XML based text files which includes coordinate system transformation matrices between joint testing and imaging coordinate systems of bones, experimental anatomical landmarks transformed to model coordinate systems, and registration error estimates.	.xml <sup>8</sup>
<b>Processed Kinematics-Kinetics Data</b>	CSV based text files storing experimental knee kinematics and kinetics processed for use in calibrated model, as loading and boundary conditions and to assess predictive capacity; supported by graphs as binary image files, including all experiment conditions.	.csv <sup>12</sup> .png <sup>13</sup>
<b>Experiment to Model File</b>	Describes which processed kinematics and kinetics experimental data was used to generate a model to mimic experimental conditions. (used as input for model generation and post processing scripts)	.xml <sup>8</sup>
<b>Optimization Results</b>	Text based files summarizing target parameters and fit error before and after calibration.	.txt
<b>Model Prediction Errors</b>	XML based text files storing experimental and model predicted knee kinematics and kinetics and errors describing correspondence between model predictions against experimental data; supported by graphs as binary image files	.xml <sup>8</sup> .png <sup>13</sup>

# Contents

## Outputs Folder Structure

Overall structure of the output folder is presented in here to facilitate navigation; listing is in alphabetical order.

```
└── CC-OKS-MC-outputs
    ├── OKS_CalibrationSummary.docx
    ├── CustomizedFullModels
    ├── └── TestSimulation
        ├── InSituStrain
        ├── MaterialProperties
        ├── Meshes
        ├── Registered
        └── └── Springs
    ├── └── ExperimentalLoading
    ├── DataProcessing
    ├── └── ProcessedData
    ├── InSituStrain
    ├── └── AnteriorLaxity
    ├── └── PosteriorLaxity
    ├── └── ValgusLaxity
    ├── └── VarusLaxity
    ├── └── InSituOpt.xml
    ├── └── ModelProperties.xml
    ├── MaterialProperties
    ├── MeshConvergence
    ├── └── geometry
    ├── └── MED
    ├── └── models
    ├── Registration
    ├── └── model
    ├── └── └── Connectivity.xml
    ├── └── └── Febio
```

```
| | | └─ MED  
| | └─ ModelProperties.xml  
| └─ check_registration.hdf  
└─ RegistrationResults_oks003.xml
```

## Outputs Folder Contents

Naming conventions for many of the subfolders and files in the outputs folder utilize the following labeling of tissue types:

- **FMC**: femoral cartilage
- **TBC-M**: medial tibial cartilage
- **TBC-L**: lateral tibial cartilage
- **PTC**: patellar cartilage
- **MNS-M**: medial meniscus
- **MNS-L**: lateral meniscus
- **ACL**: anterior cruciate ligament
- **PCL**: posterior cruciate ligament
- **MCL**: medial collateral ligament
- **LCL**: lateral collateral ligament
- **PTL**: patellar ligament
- **QAT**: quadriceps tendon

Contents of subfolders of the outputs folder are described below, in the order that they appear in the model development specifications<sup>1</sup>.

### **./MeshConvergence**

The MeshConvergence folder contains geometries, meshes, and models used in the mesh convergence process.

**./MeshConvergence/geometry**

The geometry folder contains the geometry files used to build the meshes at varying mesh densities. Naming convention used for the geometry files includes the name of the specimen (oks003), the tissue type, and the sampling rate used in ISO parameterization remeshing.

For example, oks003\_MCL\_IP5.stl is a geometry file from the Open Knee(s) specimen, of the medial collateral ligament, remeshed at a sampling rate of 5.

The files included in the geometry folder are:

oks003\_ACL\_IP4.stl

oks003\_ACL\_IP6.stl

oks003\_ACL\_IP8.stl

oks003\_ACL\_IP10.stl

oks003\_ACL\_IP12.stl

oks003\_ACL\_IP14.stl

oks003\_FMC\_IP8.stl

oks003\_FMC\_IP10.stl

oks003\_FMC\_IP12.stl

oks003\_FMC\_IP15.stl

oks003\_LCL\_IP3.stl

oks003\_LCL\_IP4.stl

oks003\_LCL\_IP6.stl

oks003\_LCL\_IP8.stl

oks003\_MCL\_IP5.stl

oks003\_MCL\_IP7.stl

oks003\_MCL\_IP9.stl

oks003\_MCL\_IP11.stl

oks003\_MNS-L\_IP4.stl

oks003\_MNS-L\_IP6.stl

oks003\_MNS-L\_IP8.stl

oks003\_MNS-L\_IP10.stl

oks003\_MNS-L\_IP12.stl

oks003\_MNS-L\_IP14.stl

oks003\_MNS-M\_IP4.stl

oks003\_MNS-M\_IP6.stl

ok003\_MNS-M\_IP8.stl

ok003\_MNS-M\_IP10.stl

ok003\_MNS-M\_IP12.stl

ok003\_PCL\_IP3.stl

ok003\_PCL\_IP4.stl

ok003\_PCL\_IP6.stl

ok003\_PCL\_IP8.stl

ok003\_PTC\_IP6.stl

ok003\_PTC\_IP8.stl

ok003\_PTC\_IP10.stl

ok003\_PTC\_IP12.stl

ok003\_PTL\_IP4.stl

ok003\_PTL\_IP6.stl

ok003\_PTL\_IP8.stl

ok003\_PTL\_IP10.stl

ok003\_QAT\_IP4.stl

ok003\_QAT\_IP6.stl

ok003\_QAT\_IP8.stl

ok003\_QAT\_IP10.stl

ok003\_TBC-L\_IP6.stl

ok003\_TBC-L\_IP8.stl

ok003\_TBC-L\_IP10.stl

ok003\_TBC-L\_IP12.stl

ok003\_TBC-M\_IP6.stl

ok003\_TBC-M\_IP8.stl

ok003\_TBC-M\_IP10.stl

ok003\_TBC-M\_IP12.stl

ok003\_TBC-M\_IP15.stl

## ./MeshConvergence/MED

The MED folder contains the mesh files used to build models to analyze the tissue as varying mesh densities. Naming convention used for the files in the MED folder follows the same naming convention used for the geometry files.

The files included in the MED folder are:

oks003\_ACL\_IP4.med

oks003\_ACL\_IP6.med

oks003\_ACL\_IP8.med

oks003\_ACL\_IP10.med

oks003\_ACL\_IP12.med

oks003\_ACL\_IP14.med

oks003\_FMC\_IP8.med

oks003\_FMC\_IP10.med

oks003\_FMC\_IP12.med

oks003\_FMC\_IP15.med

oks003\_LCL\_IP3.med

oks003\_LCL\_IP4.med

oks003\_LCL\_IP6.med

oks003\_LCL\_IP8.med

oks003\_MCL\_IP5.med

oks003\_MCL\_IP7.med

oks003\_MCL\_IP9.med

oks003\_MCL\_IP11.med

oks003\_MNS-L\_IP4.med

oks003\_MNS-L\_IP6.med

oks003\_MNS-L\_IP8.med

oks003\_MNS-L\_IP10.med

oks003\_MNS-L\_IP12.med

oks003\_MNS-L\_IP14.med

oks003\_MNS-M\_IP4.med  
oks003\_MNS-M\_IP6.med  
oks003\_MNS-M\_IP8.med  
oks003\_MNS-M\_IP10.med  
oks003\_MNS-M\_IP12.med  
oks003\_PCL\_IP3.med  
oks003\_PCL\_IP4.med  
oks003\_PCL\_IP6.med  
oks003\_PCL\_IP8.med  
oks003\_PTC\_IP6.med  
oks003\_PTC\_IP8.med  
oks003\_PTC\_IP10.med  
oks003\_PTC\_IP12.med  
oks003\_PTL\_IP4.med  
oks003\_PTL\_IP6.med  
oks003\_PTL\_IP8.med  
oks003\_PTL\_IP10.med  
oks003\_QAT\_IP4.med  
oks003\_QAT\_IP6.med  
oks003\_QAT\_IP8.med  
oks003\_QAT\_IP10.med  
oks003\_TBC-L\_IP6.med  
oks003\_TBC-L\_IP8.med  
oks003\_TBC-L\_IP10.med  
oks003\_TBC-L\_IP12.med  
oks003\_TBC-M\_IP6.med  
oks003\_TBC-M\_IP8.med  
oks003\_TBC-M\_IP10.med  
oks003\_TBC-M\_IP12.med

oks003\_TBC-M\_IP15.med

./MeshConvergence/models

The models folder contains the model files used to assess the tissues at varying mesh densities for each tissue of interest. The models folder contains a subfolder for each tissue of interest. The models folder also contains the Model Properties file which was used to generate all the models.

The models folder contains the following files and subfolders

ACL/

FMC/

LCL/

MCL/

MNS-L/

MNS-M/

PCL/

PTC/

PTL/

QAT/

TBC-L/

TBC-M/

ModelProperties.xml

./MeshConvergence/models/<tissue>

Each tissue folder contains a connectivity file (.xml), and a subfolder for models (Febio) at each mesh density. The connectivity file was used to assemble the models. The naming convention of the connectivity files includes the tissue type, followed by the word Connectivity, and then the sampling rate, representing mesh density. The naming convention of the Febio folders includes the word Febio followed by the sampling rate.

For example:

./MeshConvergence/models/PTC/ contains all the model files used in patellar cartilage mesh convergence

./MeshConvergence/models/PTC/PTCConnectivity\_IP6.xml is the connectivity file used to assemble the model with patella cartilage with a mesh resampled at a sampling rate of 6

./MeshConvergence/models/PTC/Febio\_IP6/ contains the model with patella cartilage with a mesh resampled at

a sampling rate of 6

Included in each of the Febio folders are:

Template model files: FeBio.feb, Geometry.feb

Customized model files: FeBio\_custom.feb, Geometry\_custom.feb

Raw simulation results: FeBio\_custom.log, FeBio\_custom.xplt

## **./MaterialProperties**

The MaterialProperties folder contains models used in the material properties confirmation process. There is one subfolder for each of the tissues assessed. The naming convention of the subfolder includes the tissue type, and the sampling rate of the mesh (converged mesh density).

The MaterialProperties folder contains the following subfolders:

ACL\_IP8/

LCL\_IP6/

MCL\_IP7/

PCL\_IP6/

QAT\_IP6/

TBC-L\_IP6/

Each of the subfolders above contain the following model files:

Customized model files: FeBio\_custom.feb, Geometry\_custom.feb

Raw simulation results: FeBio\_custom.log, FeBio\_custom.xplt

## **./Registration**

The Registration folder contains:

Salome file used to visualize registration results against bone geometries: check\_registration.hdf

Results of registration: RegistrationResults\_oks003.xml

./Registration/model/

The model folder contains all the files used to generate the registered model including:

The connectivity file: Connectivity.xml

The model properties file, including converged material properties, and registered anatomical axes: ModelProperties.xml

./Registraiton/model/MED

The MED folder contains all the meshes at the converged mesh densities used to build the registered model.

oks003\_ACL\_IP8.med

oks003\_FBB\_AGS\_LVTIT.med

oks003\_FMB\_AGS\_LVTIT.med

oks003\_FMC\_IP12.med

oks003\_MCL\_IP7.med

oks003\_MNS-L\_IP8.med

oks003\_MNS-M\_IP10.med

oks003\_PCL\_IP6.med

oks003\_PT\_BAGS\_LVTIT.med

oks003\_PTC\_IP6.med

oks003\_PTL\_IP6.med

oks003\_QAT\_IP6.med

oks003\_TBB\_AGS\_LVTIT.med

oks003\_TBC-L\_IP6.med

oks003\_TBC-M\_IP10.med

./Registraiton/model/Febio

The Febio folder contains the registered model files. The customized model files with mcltie in the name represent models where a tie contact was used between the mcl and mns-m. Those without mcltie in the name represent models where springs were used to connect the mcl to the mns-m. Details in protocol deviations.

Template model files: FeBio.feb, Geometry.feb

Customized model files: FeBio\_custom.feb, Geometry\_custom.feb, FeBio\_custom\_mcltie.feb, Geometry\_custom\_mcltie.feb

## ./DataProcessing

./DataProcessing/ProcessedData/

Naming conventions are described in the readme.txt file, the ProcessedData folder contains the following files:

Laxity\_0deg\_AP1\_kinematics\_in\_JCS.csv

Laxity\_0deg\_AP1\_kinematics\_in\_JCS.png

Laxity\_0deg\_AP1\_kinematics\_in\_JCS\_experiment.csv

Laxity\_0deg\_AP1\_kinematics\_in\_JCS\_experiment.png

Laxity\_0deg\_AP1\_kinetics\_in\_ImageCS.csv

Laxity\_0deg\_AP1\_kinetics\_in\_TibiaCS.csv

Laxity\_0deg\_AP1\_kinetics\_in\_TibiaCS.png

Laxity\_0deg\_AP1\_TibiaKinetics\_in\_TibiaCS.csv

Laxity\_0deg\_AP1\_TibiaKinetics\_in\_TibiaCS.png

Laxity\_0deg\_AP2\_kinematics\_in\_JCS.csv

Laxity\_0deg\_AP2\_kinematics\_in\_JCS.png

Laxity\_0deg\_AP2\_kinematics\_in\_JCS\_experiment.csv

Laxity\_0deg\_AP2\_kinematics\_in\_JCS\_experiment.png

Laxity\_0deg\_AP2\_kinetics\_in\_ImageCS.csv

Laxity\_0deg\_AP2\_kinetics\_in\_TibiaCS.csv

Laxity\_0deg\_AP2\_kinetics\_in\_TibiaCS.png

Laxity\_0deg\_AP2\_TibiaKinetics\_in\_TibiaCS.csv

Laxity\_0deg\_AP2\_TibiaKinetics\_in\_TibiaCS.png

Laxity\_0deg\_EI1\_kinematics\_in\_JCS.csv

Laxity\_0deg\_EI1\_kinematics\_in\_JCS.png

Laxity\_0deg\_EI1\_kinematics\_in\_JCS\_experiment.csv

Laxity\_0deg\_EI1\_kinematics\_in\_JCS\_experiment.png

Laxity\_0deg\_EI1\_kinetics\_in\_ImageCS.csv

Laxity\_0deg\_EI1\_kinetics\_in\_TibiaCS.csv

Laxity\_0deg\_EI1\_kinetics\_in\_TibiaCS.png

Laxity\_0deg\_EI1\_TibiaKinetics\_in\_TibiaCS.csv  
Laxity\_0deg\_EI1\_TibiaKinetics\_in\_TibiaCS.png  
Laxity\_0deg\_EI2\_kinematics\_in\_JCS.csv  
Laxity\_0deg\_EI2\_kinematics\_in\_JCS.png  
Laxity\_0deg\_EI2\_kinematics\_in\_JCS\_experiment.csv  
Laxity\_0deg\_EI2\_kinematics\_in\_JCS\_experiment.png  
Laxity\_0deg\_EI2\_kinetics\_in\_ImageCS.csv  
Laxity\_0deg\_EI2\_kinetics\_in\_TibiaCS.csv  
Laxity\_0deg\_EI2\_kinetics\_in\_TibiaCS.png  
Laxity\_0deg\_EI2\_TibiaKinetics\_in\_TibiaCS.csv  
Laxity\_0deg\_EI2\_TibiaKinetics\_in\_TibiaCS.png  
Laxity\_0deg\_Kinematics\_raw.csv  
Laxity\_0deg\_Kinematics\_raw.png  
Laxity\_0deg\_Kinetics\_raw.csv  
Laxity\_0deg\_Kinetics\_raw.png  
Laxity\_0deg\_VV1\_kinematics\_in\_JCS.csv  
Laxity\_0deg\_VV1\_kinematics\_in\_JCS.png  
Laxity\_0deg\_VV1\_kinematics\_in\_JCS\_experiment.csv  
Laxity\_0deg\_VV1\_kinematics\_in\_JCS\_experiment.png  
Laxity\_0deg\_VV1\_kinetics\_in\_ImageCS.csv  
Laxity\_0deg\_VV1\_kinetics\_in\_TibiaCS.csv  
Laxity\_0deg\_VV1\_kinetics\_in\_TibiaCS.png  
Laxity\_0deg\_VV1\_TibiaKinetics\_in\_TibiaCS.csv  
Laxity\_0deg\_VV1\_TibiaKinetics\_in\_TibiaCS.png  
Laxity\_0deg\_VV2\_kinematics\_in\_JCS.csv  
Laxity\_0deg\_VV2\_kinematics\_in\_JCS.png  
Laxity\_0deg\_VV2\_kinematics\_in\_JCS\_experiment.csv  
Laxity\_0deg\_VV2\_kinematics\_in\_JCS\_experiment.png  
Laxity\_0deg\_VV2\_kinetics\_in\_ImageCS.csv

Laxity\_0deg\_VV2\_kinetics\_in\_TibiaCS.csv  
Laxity\_0deg\_VV2\_kinetics\_in\_TibiaCS.png  
Laxity\_0deg\_VV2\_TibiaKinetics\_in\_TibiaCS.csv  
Laxity\_0deg\_VV2\_TibiaKinetics\_in\_TibiaCS.png  
Laxity\_30deg\_AP1\_kinematics\_in\_JCS.csv  
Laxity\_30deg\_AP1\_kinematics\_in\_JCS.png  
Laxity\_30deg\_AP1\_kinematics\_in\_JCS\_experiment.csv  
Laxity\_30deg\_AP1\_kinematics\_in\_JCS\_experiment.png  
Laxity\_30deg\_AP1\_kinetics\_in\_ImageCS.csv  
Laxity\_30deg\_AP1\_kinetics\_in\_TibiaCS.csv  
Laxity\_30deg\_AP1\_kinetics\_in\_TibiaCS.png  
Laxity\_30deg\_AP1\_TibiaKinetics\_in\_TibiaCS.csv  
Laxity\_30deg\_AP1\_TibiaKinetics\_in\_TibiaCS.png  
Laxity\_30deg\_AP2\_kinematics\_in\_JCS.csv  
Laxity\_30deg\_AP2\_kinematics\_in\_JCS.png  
Laxity\_30deg\_AP2\_kinematics\_in\_JCS\_experiment.csv  
Laxity\_30deg\_AP2\_kinematics\_in\_JCS\_experiment.png  
Laxity\_30deg\_AP2\_kinetics\_in\_ImageCS.csv  
Laxity\_30deg\_AP2\_kinetics\_in\_TibiaCS.csv  
Laxity\_30deg\_AP2\_kinetics\_in\_TibiaCS.png  
Laxity\_30deg\_AP2\_TibiaKinetics\_in\_TibiaCS.csv  
Laxity\_30deg\_AP2\_TibiaKinetics\_in\_TibiaCS.png  
Laxity\_30deg\_EI1\_kinematics\_in\_JCS.csv  
Laxity\_30deg\_EI1\_kinematics\_in\_JCS.png  
Laxity\_30deg\_EI1\_kinematics\_in\_JCS\_experiment.csv  
Laxity\_30deg\_EI1\_kinematics\_in\_JCS\_experiment.png  
Laxity\_30deg\_EI1\_kinetics\_in\_ImageCS.csv  
Laxity\_30deg\_EI1\_kinetics\_in\_TibiaCS.csv  
Laxity\_30deg\_EI1\_kinetics\_in\_TibiaCS.png

Laxity\_30deg\_EI1\_TibiaKinetics\_in\_TibiaCS.csv

Laxity\_30deg\_EI1\_TibiaKinetics\_in\_TibiaCS.png

Laxity\_30deg\_EI2\_kinematics\_in\_JCS.csv

Laxity\_30deg\_EI2\_kinematics\_in\_JCS.png

Laxity\_30deg\_EI2\_kinematics\_in\_JCS\_experiment.csv

Laxity\_30deg\_EI2\_kinematics\_in\_JCS\_experiment.png

Laxity\_30deg\_EI2\_kinetics\_in\_ImageCS.csv

Laxity\_30deg\_EI2\_kinetics\_in\_TibiaCS.csv

Laxity\_30deg\_EI2\_kinetics\_in\_TibiaCS.png

Laxity\_30deg\_EI2\_TibiaKinetics\_in\_TibiaCS.csv

Laxity\_30deg\_EI2\_TibiaKinetics\_in\_TibiaCS.png

Laxity\_30deg\_Kinematics\_raw.csv

Laxity\_30deg\_Kinematics\_raw.png

Laxity\_30deg\_Kinetics\_raw.csv

Laxity\_30deg\_Kinetics\_raw.png

Laxity\_30deg\_VV1\_kinematics\_in\_JCS.csv

Laxity\_30deg\_VV1\_kinematics\_in\_JCS.png

Laxity\_30deg\_VV1\_kinematics\_in\_JCS\_experiment.csv

Laxity\_30deg\_VV1\_kinematics\_in\_JCS\_experiment.png

Laxity\_30deg\_VV1\_kinetics\_in\_ImageCS.csv

Laxity\_30deg\_VV1\_kinetics\_in\_TibiaCS.csv

Laxity\_30deg\_VV1\_kinetics\_in\_TibiaCS.png

Laxity\_30deg\_VV1\_TibiaKinetics\_in\_TibiaCS.csv

Laxity\_30deg\_VV1\_TibiaKinetics\_in\_TibiaCS.png

Laxity\_30deg\_VV2\_kinematics\_in\_JCS.csv

Laxity\_30deg\_VV2\_kinematics\_in\_JCS.png

Laxity\_30deg\_VV2\_kinematics\_in\_JCS\_experiment.csv

Laxity\_30deg\_VV2\_kinematics\_in\_JCS\_experiment.png

Laxity\_30deg\_VV2\_kinetics\_in\_ImageCS.csv

Laxity\_30deg\_VV2\_kinetics\_in\_TibiaCS.csv  
Laxity\_30deg\_VV2\_kinetics\_in\_TibiaCS.png  
Laxity\_30deg\_VV2\_TibiaKinetics\_in\_TibiaCS.csv  
Laxity\_30deg\_VV2\_TibiaKinetics\_in\_TibiaCS.png  
Laxity\_60deg\_AP1\_kinematics\_in\_JCS.csv  
Laxity\_60deg\_AP1\_kinematics\_in\_JCS.png  
Laxity\_60deg\_AP1\_kinematics\_in\_JCS\_experiment.csv  
Laxity\_60deg\_AP1\_kinematics\_in\_JCS\_experiment.png  
Laxity\_60deg\_AP1\_kinetics\_in\_ImageCS.csv  
Laxity\_60deg\_AP1\_kinetics\_in\_TibiaCS.csv  
Laxity\_60deg\_AP1\_kinetics\_in\_TibiaCS.png  
Laxity\_60deg\_AP1\_TibiaKinetics\_in\_TibiaCS.csv  
Laxity\_60deg\_AP1\_TibiaKinetics\_in\_TibiaCS.png  
Laxity\_60deg\_AP2\_kinematics\_in\_JCS.csv  
Laxity\_60deg\_AP2\_kinematics\_in\_JCS.png  
Laxity\_60deg\_AP2\_kinematics\_in\_JCS\_experiment.csv  
Laxity\_60deg\_AP2\_kinematics\_in\_JCS\_experiment.png  
Laxity\_60deg\_AP2\_kinetics\_in\_ImageCS.csv  
Laxity\_60deg\_AP2\_kinetics\_in\_TibiaCS.csv  
Laxity\_60deg\_AP2\_kinetics\_in\_TibiaCS.png  
Laxity\_60deg\_AP2\_TibiaKinetics\_in\_TibiaCS.csv  
Laxity\_60deg\_AP2\_TibiaKinetics\_in\_TibiaCS.png  
Laxity\_60deg\_EI1\_kinematics\_in\_JCS.csv  
Laxity\_60deg\_EI1\_kinematics\_in\_JCS.png  
Laxity\_60deg\_EI1\_kinematics\_in\_JCS\_experiment.csv  
Laxity\_60deg\_EI1\_kinematics\_in\_JCS\_experiment.png  
Laxity\_60deg\_EI1\_kinetics\_in\_ImageCS.csv  
Laxity\_60deg\_EI1\_kinetics\_in\_TibiaCS.csv  
Laxity\_60deg\_EI1\_kinetics\_in\_TibiaCS.png

Laxity\_60deg\_EI1\_TibiaKinetics\_in\_TibiaCS.csv

Laxity\_60deg\_EI1\_TibiaKinetics\_in\_TibiaCS.png

Laxity\_60deg\_EI2\_kinematics\_in\_JCS.csv

Laxity\_60deg\_EI2\_kinematics\_in\_JCS.png

Laxity\_60deg\_EI2\_kinematics\_in\_JCS\_experiment.csv

Laxity\_60deg\_EI2\_kinematics\_in\_JCS\_experiment.png

Laxity\_60deg\_EI2\_kinetics\_in\_ImageCS.csv

Laxity\_60deg\_EI2\_kinetics\_in\_TibiaCS.csv

Laxity\_60deg\_EI2\_kinetics\_in\_TibiaCS.png

Laxity\_60deg\_EI2\_TibiaKinetics\_in\_TibiaCS.csv

Laxity\_60deg\_EI2\_TibiaKinetics\_in\_TibiaCS.png

Laxity\_60deg\_Kinematics\_raw.csv

Laxity\_60deg\_Kinematics\_raw.png

Laxity\_60deg\_Kinetics\_raw.csv

Laxity\_60deg\_Kinetics\_raw.png

Laxity\_60deg\_VV1\_kinematics\_in\_JCS.csv

Laxity\_60deg\_VV1\_kinematics\_in\_JCS.png

Laxity\_60deg\_VV1\_kinetics\_in\_ImageCS.csv

Laxity\_60deg\_VV1\_kinetics\_in\_TibiaCS.csv

Laxity\_60deg\_VV1\_kinetics\_in\_TibiaCS.png

Laxity\_60deg\_VV1\_TibiaKinetics\_in\_TibiaCS.csv

Laxity\_60deg\_VV1\_TibiaKinetics\_in\_TibiaCS.png

Laxity\_60deg\_VV2\_kinematics\_in\_JCS.csv

Laxity\_60deg\_VV2\_kinematics\_in\_JCS.png

Laxity\_60deg\_VV2\_kinematics\_in\_JCS\_experiment.csv

Laxity\_60deg\_VV2\_kinematics\_in\_JCS\_experiment.png

Laxity\_60deg\_VV2\_kinetics\_in\_ImageCS.csv

Laxity\_60deg\_VV2\_kinetics\_in\_TibiaCS.csv

Laxity\_60deg\_VV2\_kinetics\_in\_TibiaCS.png

Laxity\_60deg\_VV2\_TibiaKinetics\_in\_TibiaCS.csv

Laxity\_60deg\_VV2\_TibiaKinetics\_in\_TibiaCS.png

Laxity\_90deg\_AP1\_kinematics\_in\_JCS.csv

Laxity\_90deg\_AP1\_kinematics\_in\_JCS.png

Laxity\_90deg\_AP1\_kinematics\_in\_JCS\_experiment.csv

Laxity\_90deg\_AP1\_kinematics\_in\_JCS\_experiment.png

Laxity\_90deg\_AP1\_kinetics\_in\_ImageCS.csv

Laxity\_90deg\_AP1\_kinetics\_in\_TibiaCS.csv

Laxity\_90deg\_AP1\_kinetics\_in\_TibiaCS.png

Laxity\_90deg\_AP1\_TibiaKinetics\_in\_TibiaCS.csv

Laxity\_90deg\_AP1\_TibiaKinetics\_in\_TibiaCS.png

Laxity\_90deg\_AP2\_kinematics\_in\_JCS.csv

Laxity\_90deg\_AP2\_kinematics\_in\_JCS.png

Laxity\_90deg\_AP2\_kinematics\_in\_JCS\_experiment.csv

Laxity\_90deg\_AP2\_kinematics\_in\_JCS\_experiment.png

Laxity\_90deg\_AP2\_kinetics\_in\_ImageCS.csv

Laxity\_90deg\_AP2\_kinetics\_in\_TibiaCS.csv

Laxity\_90deg\_AP2\_kinetics\_in\_TibiaCS.png

Laxity\_90deg\_AP2\_TibiaKinetics\_in\_TibiaCS.csv

Laxity\_90deg\_AP2\_TibiaKinetics\_in\_TibiaCS.png

Laxity\_90deg\_EI1\_kinematics\_in\_JCS.csv

Laxity\_90deg\_EI1\_kinematics\_in\_JCS.png

Laxity\_90deg\_EI1\_kinematics\_in\_JCS\_experiment.csv

Laxity\_90deg\_EI1\_kinematics\_in\_JCS\_experiment.png

Laxity\_90deg\_EI1\_kinetics\_in\_ImageCS.csv

Laxity\_90deg\_EI1\_kinetics\_in\_TibiaCS.csv

Laxity\_90deg\_EI1\_kinetics\_in\_TibiaCS.png

Laxity\_90deg\_EI1\_TibiaKinetics\_in\_TibiaCS.csv

Laxity\_90deg\_EI1\_TibiaKinetics\_in\_TibiaCS.png

Laxity\_90deg\_EI2\_kinematics\_in\_JCS.csv  
Laxity\_90deg\_EI2\_kinematics\_in\_JCS.png  
Laxity\_90deg\_EI2\_kinematics\_in\_JCS\_experiment.csv  
Laxity\_90deg\_EI2\_kinematics\_in\_JCS\_experiment.png  
Laxity\_90deg\_EI2\_kinetics\_in\_ImageCS.csv  
Laxity\_90deg\_EI2\_kinetics\_in\_TibiaCS.csv  
Laxity\_90deg\_EI2\_kinetics\_in\_TibiaCS.png  
Laxity\_90deg\_EI2\_TibiaKinetics\_in\_TibiaCS.csv  
Laxity\_90deg\_EI2\_TibiaKinetics\_in\_TibiaCS.png  
Laxity\_90deg\_Kinematics\_raw.csv  
Laxity\_90deg\_Kinematics\_raw.png  
Laxity\_90deg\_Kinetics\_raw.csv  
Laxity\_90deg\_Kinetics\_raw.png  
Laxity\_90deg\_VV1\_kinematics\_in\_JCS.csv  
Laxity\_90deg\_VV1\_kinematics\_in\_JCS.png  
Laxity\_90deg\_VV1\_kinematics\_in\_JCS\_experiment.csv  
Laxity\_90deg\_VV1\_kinematics\_in\_JCS\_experiment.png  
Laxity\_90deg\_VV1\_kinetics\_in\_ImageCS.csv  
Laxity\_90deg\_VV1\_kinetics\_in\_TibiaCS.csv  
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Laxity\_90deg\_VV1\_TibiaKinetics\_in\_TibiaCS.csv  
Laxity\_90deg\_VV1\_TibiaKinetics\_in\_TibiaCS.png  
Laxity\_90deg\_VV2\_kinematics\_in\_JCS.csv  
Laxity\_90deg\_VV2\_kinematics\_in\_JCS.png  
Laxity\_90deg\_VV2\_kinematics\_in\_JCS\_experiment.csv  
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Laxity\_90deg\_VV2\_kinetics\_in\_ImageCS.csv  
Laxity\_90deg\_VV2\_kinetics\_in\_TibiaCS.csv  
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Laxity\_90deg\_VV2\_TibiaKinetics\_in\_TibiaCS.csv  
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Passive\_Flexion\_Kinematics\_in\_JCS.csv  
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Passive\_Flexion\_kinematics\_in\_JCS\_experiment.csv  
Passive\_Flexion\_kinematics\_in\_JCS\_experiment.png  
Passive\_Flexion\_Kinematics\_raw.csv  
Passive\_Flexion\_Kinematics\_raw.png  
Passive\_Flexion\_Kinetics\_in\_ImageCS.csv  
Passive\_Flexion\_Kinetics\_in\_TibiaCS.csv  
Passive\_Flexion\_Kinetics\_in\_TibiaCS.png  
Passive\_Flexion\_Kinetics\_raw.csv  
Passive\_Flexion\_Kinetics\_raw.png  
Readme.txt

## **/InSituStrain**

InSituStrain folder contains:

InSituOpt.xml – file used to run the optimization script

ModelProperties.xml used for post processing during optimization

One folder for each of the laxity models used in optimization of in situ strains.

`./InSituStrain/<laxity model>`

Each of the laxity model folders contains:

Customized model files of that last attempted in situ strain value during optimization: FeBio\_custom.feb, Geometry\_custom.feb

Raw simulation results of that last attempted in situ strain value during optimization: FeBio\_custom.log, FeBio\_custom.xplt

Optimization Results files: Optimization<n>.txt

Processed simulation results of that last attempted in situ strain value during optimization: `./InSituStrain/<laxity model>/Processed_Results`

Each Processed Results folder contains the following files:

Tibia\_Translation.csv

Tibiofemoral\_Kinematics.csv

Tibiofemoral\_Kinetics.csv

## /CustomizedFullModels

./CustomizedFullModels/ExperimentalLoading

The ExperimentalLoading folder contains all the customized model files and raw simulations results to replicate experimental loading. For each model there is a folder containing the post-processed model results. Naming convention for the models is described in the calibration specifications and protocol deviations.

The following is a list of the files contained in ExperimentalLoading which are not defined in previous documentation:

Experiment to Model File: Exp\_to\_Mod.xml

Initial customized model used to create all experimental loading cases: FeBio\_custom.feb, Geometry\_custom.feb

Model properties file: ModelProperties.xml

./CustomizedFullModels/ExperimentalLoading/Processed\_Results\_<model name>/

The Processed\_Results folder contains the model post-processing and model prediction error files:

JCS\_Kinematics\_Prediction\_Errors.png

JCS\_Kinematics\_Prediction\_Errors.xml

Patella\_Translation.csv

Patella\_Translation.png

Patellofemoral\_Kinematics.csv

Patellofemoral\_Kinematics.png

Tibia\_Translation.csv

Tibia\_Translation.png

Tibiofemoral\_Kinematics.csv

Tibiofemoral\_Kinematics.png

Tibiofemoral\_Kinetics.csv

## Tibiofemoral\_Kinetics.png

./CustomizedFullModels/TestSimulation

Contains model folders with staged changes to the initial working model as described in calibrations specifications and protocol deviations.

./CustomizedFullModels/TestSimulation/Springs – initial working model, with springs replacing the tied contact between the MCL and MNS-M

./CustomizedFullModels/TestSimulation/Meshes – initial working model, with springs replacing the tied contact between the MCL and MNS-M, with meshes replaced by the converged mesh densities

./CustomizedFullModels/TestSimulation/MaterialProperties - initial working model, with springs replacing the tied contact between the MCL and MNS-M, with meshes replaced by the converged mesh densities, with materials properties changed to the confirmed material properties

./CustomizedFullModels/TestSimulation/InSituStrain - initial working model, with springs replacing the tied contact between the MCL and MNS-M, with meshes replaced by the converged mesh densities, with materials properties changed to the confirmed material properties, with calibrated in situ strains

./CustomizedFullModels/TestSimulation/Registered - initial working model, with springs replacing the tied contact between the MCL and MNS-M, with meshes replaced by the converged mesh densities, with materials properties changed to the confirmed material properties, with calibrated in situ strains, registered to the experiment coordinate systems.

Each of the above folders contains the following files and subfolders:

Template model files: FeBio.feb, Geometry.feb

Customized model files: FeBio\_custom.feb, Geometry\_custom.feb

Raw simulation results: FeBio\_custom.log, FeBio\_custom.xplt

./CustomizedFullModels/TestSimulation/<staged model>/Processed\_Results:

The Processed Results folder contains the following files:

Patella\_Translation.csv

Patella\_Translation.png

Patellofemoral\_Kinematics.csv

Patellofemoral\_Kinematics.png

Tibia\_Translation.csv

Tibia\_Translation.png

Tibiofemoral\_Kinematics.csv

Tibiofemoral\_Kinematics.png

Tibiofemoral\_Kinetics.csv

Tibiofemoral\_Kinetics.png

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