Automated creation and tuning of personalised muscle paths for OpenSim musculoskeletal models via the Musculoskeletal Atlas Project Client

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Abstract

Computational modelling is an invaluable tool for investigating features of human locomotion which cannot be measured except for highly invasive techniques. Recent research has focussed on creating personalised musculoskeletal models using medical imaging. Although progress has been made, robust definition of two critical model parameters remains challenging; (i) tibiofemoral (TF) and patellofemoral (PF) joint motions, and (ii) muscle tendon unit (MTU) pathways and kinematics. The aim of this study was to develop a highly automated framework for the definition of personalised musculoskeletal models, consisting of personalised bone geometries, TF and PF joint models, and MTU pathways and kinematics. Informed from medical imaging, personalised rigid body 6 degree-of-freedom TF and PF joint models were created. Using atlas- and optimisation-based methods, personalised MTU pathways and kinematics were created with the aim of preventing MTUs penetrating bones and smooth MTU kinematics that follow literature patterns. This framework was deployed in Musculoskeletal Atlas Project Client for 6 participants, where 5 models with incremental personalisation were created. Three comparisons were made; (i) non-optimised and optimised models with non-personalised joint models; (ii) non-optimised and optimised models with personalised joint models; (iii) both aforementioned optimised models. Following optimisation, significant improvements were consistently shown in pattern similarity to literature data. Although not significant, improvements to all metrics were shown with reduced MTUs penetrating bone and increased kinematic smoothness. Comparing optimised models, no significant difference was identified for any evaluation metric, with a trend for more desirable results in the non-personalised joint models in most evaluation metrics.
Introduction

Computational models of the human musculoskeletal system enable researchers to study human biomechanics without invasive and/or expensive experiments. Research focus has been applied to rigid body musculoskeletal modelling tools, e.g., AnyBody Modeling Software AnyBody (AnyBody Technology, Aalborg, Denmark) (Damsgaard et al. 2006) or more commonly OpenSim (Delp et al. 2007; Seth et al. 2018), to estimate internal tissue loading, such as muscle tendon unit (MTU) and joint contact forces (Ackland et al. 2011; Andersen 2018; Cleather and Bull 2011; Guess et al. 2014; Konrath et al. 2017; Modenese et al. 2018; Saxby et al. 2016; Winby et al. 2009). These models typically use generic bone geometries, joint positions and orientations, and MTU pathways that are unlikely to reflect individual anatomy, even when carefully scaled (Davico et al. 2019; Kainz et al. 2017). Additionally, generic models typically contain simplified joints that are unlikely to represent *in-vivo* motion. Specifically, generic models typically include tibiofemoral (TFJ) and patellofemoral (PFJ) joints that permit a restricted number of degrees of freedom (DOF). Additionally, linear scaled models may not well represent inter-subject variation with respect to MTU moment arm magnitude, producing almost identical values across subjects despite previously reported magnitude variation (Arnold et al. 2010; Buford et al. 1997; Draganich et al. 1987; Fick 1879; Navacchia et al. 2017; Pal et al. 2007; Spoor and van Leeuwen 1992; Visser et al. 1990; Wilson and Sheehan 2009). Consequently, these models may be inappropriate to accurately estimate common outcome measures of movement simulations (Demers et al. 2014; Gerus et al. 2013; Lerner et al. 2015). To overcome these limitations, personalised models built using medical imaging can be used.

Numerous features within musculoskeletal models can be personalised, including bone geometry, segment mass and inertia, joint anatomy and kinematics, and MTU internal parameters and pathways (Saxby et al. 2019). Previous research (Gerus et al. 2013; Lerner et al. 2015) has shown the inclusion of personalised features has a significant effect on outcome variables from simulations (e.g., joint moments, and contact loading). Although several studies have presented methods to include personalised skeletal anatomy (Modenese et al. 2018; Scheys et al. 2009; Valente et al. 2017; Wesseling et al. 2016), and joint kinematic functions (Barzan et al. 2019; Brito da Luz et al. 2017; Dzialo et al. 2018; Smale et al. 2019), few studies have reported methods to define MTU pathways (Modenese et al. 2018; Scheys et al. 2009) in models with personalised bone geometry, and joint anatomy and kinematics. However, these
Methods are often highly manual in nature with no robust comparisons with, for example, cadaveric MTU kinematics, i.e., lengths and moment arms. This paper presents the development of a framework built atop the Musculoskeletal Atlas Project (MAP) Client (Zhang et al. 2014) that automates the creation of tuned personalised OpenSim musculoskeletal models with particular focus on the TFJ. Steps used to create these models are designed to automatically perform tasks typically performed manually, this automation being constrained by various algorithms to mimic manual checks performed by researchers. Additionally, all steps for model creation will utilise open-source software packages. Personalised features entail bone geometries, joint axes definitions, TFJ and PFJ kinematic models, MTU origins and insertions points, and intermediate pathways of selected lower-limb MTUs. The MAP-Client, with the developed open-source custom software, was used to generate five OpenSim models with different levels of personalisation, which were implemented and tested with the following three hypotheses. First (H1) tuning of MTU wrapping surfaces would improve MTU kinematics similarity with those reported in literature. Second (H2), wrapping-surface tuning would prevent MTUs penetrating bones, MTU polarity penalties, and MTU kinematic discontinuities. Finally, (H3) tuned models with personalised TFJ and PFJ kinematics would produce more ideal MTU kinematics compared to models with generic TFJ and PFJ kinematics.

**Methods**

**Gait data testing and magnetic resonance imaging**

Data were collected at Griffith University as part of an ongoing project (Ethics reference: PES/36/10/HREC). A subset of 6 participants were selected from a larger cohort to span a large range of age, height, and mass (Table 1). Participants had no history of musculoskeletal injury, trauma or lower-limb surgeries. Each participant provided their written and informed consent prior to undergoing comprehensive motion capture (MOCAP) and medical imaging sessions. Three-dimensional (3D) marker positions during a static calibration trial were converted from standard MOCAP format (i.e., .c3d) to standard OpenSim format (i.e., .trc) using MOtoNMS (Mantoan et al. 2015) for use in the MAP-Client.

Each participant underwent magnetic resonance imaging (MRI) of their lower-limbs at a local radiology clinic (QScan Southport, QLD, Australia) performed on the preceding or same day as the MOCAP session. Axial T₁-weighted 3D fast field echo sequences were acquired bilaterally from above the iliac crest to below the toes, while the participant lay supine in a 3 T
MRI scanner (Philips Medical Systems, Netherlands). Images were acquired using a body coil in 5 stations, ~245 slices per station, 10 mm inter-station overlap throughout, 1 mm slice thickness, and 1 mm inter-slice gap. Segmentations of the pelvis (excluding the sacrum), femur, tibia-fibula complex, and patella (bilaterally) were performed using Mimics V19 (Materialise, Leuven, Belgium). Dedicated TFJ and PFJ scans were also acquired of a randomised limb (Table 1), comprised of 3D proton density 16 channel sequences acquired from mid-thigh to below the tibial tuberosity. Images were acquired in one station (~440 slices) with 0.6 mm slice thickness, and 0.3 mm inter-slice gap. Images were used to segment distal femur, proximal tibia, and patella bones, as well as femoral, tibial, and patella cartilage surfaces, and lastly anterior cruciate (ACL), posterior cruciate (PCL), and medial collateral (MCL) ligaments.

[Table 1]

Creating personalised OpenSim models
Five different OpenSim models (Fig 1, Table 2) with varying levels of personalisation were created. Personalisation encompassed the automatic creation of MTU intermediate pathways using non-optimised and optimised wrapping surfaces, and scaled and personalised TFJ and PFJ kinematic joint models. Models were compared based on their performance in producing MTU kinematics that were (i) physiologically, and (ii) physically plausible (see below and Appendix 2).

Personalised OpenSim models were created using the MAP-Client by incorporating data from 3D MOCAP and MRI segmentations to reconstruct personalised bone geometries (Zhang et al. 2015). Bone reconstructions used a combination of principal component scaling, rigid registration, host-mesh fitting, and local mesh fitting to morph the MAP-Client mean statistical shape models to match personalised data (Bahl et al. 2019; Davico et al. 2019; Suwarganda et al. 2019).

[Table 2]

Bone geometric models reconstructed using MAP-Client were then used to customise a generic OpenSim model (Delp et al. 2007) with personalised bone geometries, joint positions, body mass, and inertial properties (Zhang et al. 2015). A personalised patella and PFJ was added, consistent with previous joint axes definitions (Arnold et al. 2010) with its location fixed with respect to the tibia. The final step in model creation was the definition of MTU pathways.
The MTU origin and insertion points were defined using an anatomical atlas (Zhang et al. 2015) i.e., SOMSO model (Marcus Sommer SOMSO Modelle, Sonneberg, Germany). This atlas contains a collection of lower-limb bones with MTU origin and insertion regions marked on the bone surface. The MAP-Client was used to generate bones that closely matched SOMSO model bones. Attachment regions of lower-limb MTUs were digitised and projected onto the MAP-Client generated SOMSO bones, and attachment region centroids were then projected to the closest node on the MAP-Client generated bone. Node indices were used within the MAP-Client workflow to define MTU origin and insertion points. The final development within the MAP-Client was definition of MTU intermediate pathways. Standard MAP-Client models used via points consistent with previous models; however, via points often introduce MTU kinematic discontinuities (Garner and Pandy 2000; Hammer et al. 2019) and non-physiological shapes (Appendix 1). To overcome these limitations and ensure consistency with recent OpenSim models (Arnold et al. 2010; Catelli et al. 2019; Rajagopal et al. 2016), wrapping surfaces were implemented.

Initial estimates of the wrapping-surface parameters, i.e., location, orientations, and dimensions, were based on visual inspection of the MAP-Client generated model and comparison with the Fullbody Model (Rajagopal et al. 2016). Wrapping-surface parameters were then defined based on anatomical regions, geometric shapes fit to anatomical regions, and the position of MTU path points, all automatically defined using the MAP-Client (i.e., Model 2). However, visual assessment revealed Model 2 produced MTU kinematics (i.e., lengths and moment arms) that were not guaranteed to be physiologically and physically plausible. Therefore, an automated optimisation of wrapping-surface geometries was developed.

Optimisation of the wrapping-surfaces’ geometry parameters was performed to produce physiologically plausible MTU kinematics and physically plausible MTU pathways. To this end, the optimisation employed pyswarm (A Python package for particle swarm optimization (PSO) with constraint support, Abraham D. Lee, https://pythonhosted.org/pyswarm/) with various mathematical objective criteria and penalty functions (See Appendix 2 for detailed explanations). The first set of objective criteria and penalty functions ensured physiologically plausible MTU kinematics. The first, a penalty function, termed polarity error, prevented moment arms inappropriately changing their mechanical actions, e.g., a flexor turning into an extensor. The second objective criteria, termed normalised gradient error, encouraged modelled moment arms to track their corresponding patterns from cadaveric data. Previous studies have reported MTU kinematics magnitude differences between cadaveric specimens,
so to retain this possibility, and allow optimisation to follow the general patterns of those in literature, MTU kinematics were represented as the gradient (change in MTU kinematic magnitude over a change in joint angle). The third objective criteria, termed smoothness, encouraged MTU kinematic patterns to be smooth and free of discontinuities.

Two penalty functions were also developed to produce *physically plausible* MTU pathways. One penalty reduced the possibility of modelled MTU pathways penetrating bones, and the second to prevent non-physical wrapping scenarios. Once wrapping-surface optimisation was complete for each participant, MAP-Client was used to generate an updated personalised model (Model 4). The final personalisation step within these models was the definition of personalised TFJ and PFJ kinematic models.

**Joint mechanism definitions and optimisation**

Two different sets of TFJ and PFJ mechanisms were created: first a scaled generic (Model 2 and 4) and the second personalised (Model 3 and 5). The scaled generic TFJ was represented as a one DOF hinge joint with anterior/posterior and superior/inferior translations prescribed as functions of TFJ flexion, defined using interpolating splines. Within the MAP-Client, TFJ translational splines were defined by determining the minimum distance between the medial and lateral condyles of the femur and tibia in neutral position (i.e., position in the MRI scanner). At each flexion angle, the anterior/posterior and superior/inferior translations which maintain this distance was determined and defined in the OpenSim model. All remaining TFJ degrees of freedom (i.e., medial/lateral translation, abduction/adduction, and internal/external rotation) were locked at zero.

Personalised TFJ and PFJ closed chain mechanisms were created from MRI segmentations (Barzan et al. 2019; Brito da Luz et al. 2017). Anatomical structures of interest (i.e., bones, cartilage, and three ligaments) were segmented from dedicated TFJ and PFJ MRI scans described above. Segmentations were imported into 3-matic V10 (Materialise, Leuven, Belgium), where surfaces and landmarks (e.g., ligament attachment points) necessary to define the closed chain joint mechanisms were identified. Anatomical landmarks and surfaces used to define these mechanisms were refined within an optimisation routine (described below) to ensure physiologically feasible solutions with secondary kinematics that highly correlated with cadaveric data (Barzan et al. 2019; Brito da Luz et al. 2017).

Joint-mechanism optimisation adjusted the mechanism-input parameters (e.g., ligament origin and insertion points, and anatomical landmarks) to produce physiological plausible joint
kinematics. This employed a similar optimisation method (Multiple Objective Particle Swarm Optimisation (Multi-Objective Particle Swarm Optimization (MOPSO) by Yarpiz, 2015). This optimisation solved the constrained joint mechanisms, thereby producing different candidate solutions, which were fitted by a series of spline functions completely describing 6 DOF TFJ motions; 1 prescribed DOF (i.e., flexion-extension), and 5 dependant DOFs (i.e., secondary kinematics). Each TFJ solution was paired with a unique PFJ mechanism solution. Pilot testing showed MTU kinematics were highly sensitive to TFJ solution, while for a given TFJ solution, PFJ solution had little effect on MTU kinematics. Thus, to determine the best candidate solution, each TFJ solution and it’s corresponding best PFJ solution based on correlation with cadaveric PFJ kinematics (Barzan et al. 2019; Brito da Luz et al. 2017) were selected. The various candidate personalised TFJ-PFJ models were then joined with the participant’s MAP-Client generated model (Model 2) yielding multiple candidate personalised OpenSim models, i.e. one Model 3 per TFJ solution.

The final personalised TFJ-PFJ solution was chosen based on evaluation metrics for each MTU’s kinematics from the candidate personalised OpenSim models (Model 3). Selected MTU (rectus femoris, vastus medialis, vastus lateralis, semimembranosus, biceps femoris long head, and medial gastrocnemius) kinematics were tested using the objective functions employed in the MTU wrapping-surface optimisation (see above and Appendix 2). Evaluation metrics for each MTU were summed for each model, and the TFJ-PFJ solution selected based on the lowest evaluation metric value. Final TFJ-PFJ functions were added to the participant’s model with MTU wrapping-surfaces (Model 2), to produce personalised, but not optimised model with personalised TFJ-PFJ models (Model 3). MTU wrapping-surface optimisation was then run to generate the final personalised model (Model 5).

**Model comparisons and MTU kinematic evaluation**

After each of model (Fig 1; Table 2) had been created MTU kinematic evaluation metrics were generated using the MTU wrapping-surface optimisation criteria; (i) number of moment arm polarity penalties, (ii) normalised MTU moment arm gradient error, (iii) number of MTU pathway bone penetration penalties, and (iv) MTU length and moment arm smoothness. Metrics were calculated for each MTU, model, and participant. For ease of comparison, MTUs were grouped: (i) quadriceps (left and right rectus femoris, vastus lateralis, vastus intermedius, and vastus medialis), (ii) hamstrings (left and right biceps femoris long and short head, semitendinosus, and semimembranosus), and (iii) extras (left and right medial and lateral gastrocnemius, sartorious, and gracilis). For each MTU metric, the frequency count (MTU
moment arm polarity penalties and MTU bone penetration penalties) and average ± standard deviation (MTU length and moment arm smoothness and moment arm gradient error) were calculated.

Although MTU metrics were calculated for each MTU and each model, three explicit comparisons were undertaken. The first compared models 2 and 4 to examine the effect of tuning MTU wrapping surfaces in models with generic TFJ and PFJ. The second comparison compared models 3 and 5 to explore the effect of tuning MTU wrapping surfaces in models with personalised TFJ and PFJ. The third compared models 4 and 5 to determine which of the models was most appropriate with respect to MTU kinematics. For each comparison, the superior model for each MTU and each metric was determined by comparing evaluation metric magnitudes, with smaller values indicating more physiologically/physically plausible MTU pathway/kinematics. Each comparison was coded as either (i) improved, (ii) worse, or (iii) no change, and the count (i.e., number of occurrences of i, ii, and iii) summed for each MTU group and all MTUs. Metric counts were compared using proportion tests to determine if differences were statistically significant (Wessa P., (2016), *Testing Population Proportion* (p-value) (v1.0.3)). To calculate z-scores, a null hypothesis of 50% was assumed and significance set at p<0.05. With respect to MTU group comparisons, total sample size was 48 (8 MTUs per group x 6 subjects), for model comparisons the total sample was 144 (8 MTUs per group x 3 groups x 6 subjects). The dominant outcome (i.e., improved, worse, or no change) was identified and tested for statistical significance.

[Fig 1]
Results

Model 2 versus Model 4

When using the non-personalised TFJ and PFJ models, wrapping-surface optimisation (Model 4) produced superior results to the non-optimised (Model 2) (Table 3). Typically, MTU length and moment arm smoothness, and moment arm gradient error (Fig 2 and 3) improved following MTU wrapping-surface optimisation. Model 4 performed better for several MTU metrics, although differences did not always reach statistical significance. For all MTU groups, both MTU moment arm polarity penalties and length smoothness showed no change for a significant proportion of cases. Similarly, the all MTU group, quadriceps, and hamstrings groups showed no change with respect to MTU bone penetration penalties in a significant proportion of cases. Finally, moment arm gradient error was reduced in a significant proportion of cases in all MTU groups following optimisation.

A number of non-significant trends were also observed, all indicating improvement in MTU metrics following wrapping-surface optimisation. For all MTU groups and in all metrics, except MTU moment arm smoothness, more cases of improvements (compared to cases of worsening) were observed following MTU wrapping-surface optimisation. Additionally, MTU moment arm smoothness showed a non-significant higher number of improved cases for hamstrings and extras MTU groups.

[Table 3]

[Fig 2]

[Fig 3]
Models 3 versus Model 5

Comparison of models with personalised joint kinematic models with non-optimised (Model 3) and optimised (Model 5) wrapping-surfaces revealed a significant proportion of no change cases (Table 4). The exception was MTU moment arm gradient error which, across all MTU groups, showed a significant proportion of improved cases following optimisation.

Although MTU moment arm polarity penalty showed a significant proportion of no change for the all MTU, quadriceps, and extras groups, a larger proportion (albeit not significant) of improvements (compared to worse cases) were shown following optimisation.

Similarly, MTU bone penetrations penalties showed a significant proportion of cases with no change for the all MTU, quadriceps, and hamstrings groups. Again, a larger non-significant proportion of cases showed improvement (compared to worse cases) following optimisation.

Finally, no significant proportion was found with respect to MTU moment arm smoothness, however, larger non-significant proportion of cases showed improvement (compared to worse cases) following optimisation.

[Table 4]
Models 4 vs 5

The final comparison between optimised models with generic (Model 4) and personalised (Model 5) joints showed inconsistent results (Table 5; Fig 4 and 5). Across all subjects, a significant proportion of cases for all MTU, quadriceps, and hamstrings groups showed no change between models for MTU moment arm polarity penalties. Although not significant, a larger proportion of cases showed improvements in Model 5 compared to Model 4 for the all MTU, hamstrings and extras groups. MTU bone penetration penalties showed no change between models for the all MTU, quadriceps and hamstrings groups. Unlike MTU polarity penalties, a larger non-significant proportion of cases were improved in Model 4 compared to Model 5. Length smoothness showed a significant proportion of cases with no change between models for the all MTU, hamstrings, and extras groups. Quadriceps and all MTU groups showed a larger non-significant proportion of improvements in Model 4, the extras MTU group showed a larger non-significant proportion of improvement in Model 5. Unlike previous comparisons, no significant difference was identified with respect to MTU moment arm gradient error. Although not statistically significant, improvements were shown in Model 4 compared to Model 5 in all MTU, hamstrings, and extras groups with quadriceps group showing an equal proportion of improved results for Model 4 and 5.

[Table 5]

[Fig 4]

[Fig 5]
Discussion
This study aimed to design and test a framework, built atop the MAP-Client, for the automated and tuned creation of personalised OpenSim models. The open-source framework developed provides an efficient workflow for generation of personalised OpenSim musculoskeletal model, and lends itself to many applications including personalised rehabilitation, virtual surgery outcome testing, and other clinical and sporting applications. The presented workflow automated various tasks previously performed manually or semi-manually. This was achieved by representing manual checks as mathematical algorithms that automatically detected and adjusted the models without the need for time consuming manual interventions. Additionally, all steps following MRI segmentations were performed using open-source software packages.

Generally, following optimisation, a majority of MTU evaluation metrics showed improvements in models with both generic (Model 2 and 4) and personalised (Model 3 and 5) joint models. However, a number of the improvements observed were not statistically significant and must be interpreted with caution.

The first hypothesis ($H_1$) was confirmed where in both optimised models (Model 4 and Model 5) the similarity to cadaveric literature data was improved compared to the non-optimised models (Models 2 and 3). This was represented in the results (Table 3 and 4) where moment arm gradient error was reduced in all MTU groups. This result provides confidence that the design optimisation resulted in more physiological MTU moment arms compared to non-optimised models.

The second hypothesis ($H_2$) was largely confirmed whereby, following optimisation a number of non-physiological and non-physical MTU kinematics and pathways were improved. For both comparisons (generic and personalised joints) MTU moment arm polarity penalties, MTU bone penetration penalties, and length smoothness all showed a significant proportion of no change cases between models. While several cases showed no change, the methods used do not take into account cases where no errors were present in the non-optimised model. Despite this, a non-significant trend of improvement in these metrics following optimisation was observed for all MTU groups. Similarly, a non-significant proportion of improvements was observed in moment arm smoothness for the all MTU, hamstrings, and extras groups with the quadriceps MTU group showing an equal distribution of worse and improved cases. Although MTU moment arm smoothness was included explicitly within the optimisation, and therefore should have decreased, as the optimisation minimises a single weighted objective function, a
reduction in all MTU metrics was not always achieved. In a number of cases where worse MTU moment arm smoothness was observed, changes were often small and coupled with much larger reduction in other metrics (i.e., MTU moment arm gradient error). Importantly, there were no cases that showed a statistically significant results or non-significant trend towards worse results following optimisation, providing confidence in the developed framework. These results were identical in both comparisons with the exception of a trend towards improved MTU moment arm smoothness in the extras MTU group shown in the personalised joint models (Model 5) while Model 4 showed no trend. Although a number of results were non-significant, when viewing the final performance criteria for each objective and penalty function, the desired effect was shown in a majority of cases for both Model 4 (Table 6) and Model 5 (Table 7). Performance criteria for Model 1, 2, and 3 are shown in Appendix 3.

[Table 6]

Although optimisation largely had the desired effect in Model 2, specific MTUs still exhibited undesirable features. Following optimisation, gastrocnemii MTUs often had polarity penalties at the end range of motion. To produce gastrocnemii MTU moment arms and lengths with patterns consistent with cadaveric data, they must shorten throughout TFJ flexion. Due to geometrical constraints caused by the simplified TFJ model this was not always achieved. When both the linear scaled generic and MAP-Client generated OpenSim model TFJs are flexed ≥80°, the cause of the MTU kinematic disturbance becomes apparent. The MAP-Client model tibia is translated more superiorly compared to the generic scaled model (Fig 6). Wrapping surfaces are positioned on the proximal tibia to prevent MTU penetration into the femur and tibia. The presence of these wrapping surfaces means the gastrocnemii MTUs take a more curved pathway within the MAP-Client model compared to the generic model to prevent penetration at ≥80° of TFJ flexion. This creates a scenario where, gastrocnemii MTUs lengthen with increasing flexion, hence appearing to an extensor and creating a polarity error in the MTU moment arm. Although presenting as an error within the MTU kinematic curves, the solution to this problem is a more accurate TFJ model, rather than a change to wrapping surface configuration. With the inclusion of personalised TFJ and PFJ mechanisms (Model 5), these geometric constraints are reduced, allowing for more appropriate MTU kinematics.

[Table 7]

The final hypothesis (H₃) showed varied results between the two tested models (Model 4 and 5). MTU bone penetration penalties, length smoothness, and moment arm polarity penalties,
all showed a significant proportion of no change between models in all MTU groups. No significant difference between proportions of each of the three options was shown for moment arm smoothness and gradient error. Despite this, numerous non-significant trends were observed when comparing only results that improved or worsened. Generally, MTU moment arm polarity penalties were reduced in Model 5 compared to Model 4 across all MTU groups.

[Fig 6]

Additionally, length smoothness was generally lower in the extras MTU group, again potentially due to the errors introduced by the simplified TFJ in Model 4. No clear pattern was observed for MTU moment arm smoothness comparisons, as outcomes were almost equally distributed in all MTU groups. MTU bone penetration penalties, moment arm gradient error, and length smoothness were all typically superior (albeit non-significant) in Model 4 with simplified TFJ and PFJ models. Differences in Model 4 compared to Model 5 are likely due to the simplified joint models. TFJ kinematics estimated using simplified methods show low inter-subject variability in the kinematic magnitudes and patterns (Fig 7). Conversely, personalised TFJ (Fig 8) and PFJ (Fig 9) kinematics show high inter-subject variability both in magnitude and patterns. In addition to high inter-subject variability, Model 5 permits PFJ motions likely further contributing to differences in MTU kinematics. More complex TFJ and PFJ kinematics such as those used in Model 5, likely result in more variable MTU pathways. The use of multi-planar TFJ and PFJ may require MTU wrapping-surface configurations (e.g., position, and orientation) that are vastly different compared to models with simplified joint models. Furthermore, these more complex models may require additional wrapping surfaces to constrain MTU pathways when other DOFs (e.g., abduction/adduction) are mobilised.

[Fig 7]

[Fig 8]

[Fig 9]

There are limitations to this study. The primary limitation within this study was it only considered MTU kinematics with respect to a single DOF, i.e., TFJ flexion/extension despite some MTUs being bi-articulate (e.g., rectus femoris). This means, for the considered DOF the MTU kinematics follow the pattern of cadaveric literature data; however when other DOFs are mobilised the MTU kinematics may still present with discontinuities or other observed errors. While this is acknowledged as a limitation, the designed framework was the first of its kind,
the decision to evaluate the framework on a single DOF was made. Future work will extend this framework to multiple DOFs and joints simultaneously within the optimisation framework. The second limitation within this study is related to the personalised TFJ and PFJ kinematic models. Although these models potentially produce more physiological kinematics compared to previous methods (Delp et al. 2007; Kainz et al. 2017; Modenese et al. 2018), the resulting kinematics have not been extensively validated. Although the tuning of these mechanisms ensures physiologically and physically plausible solutions that highly correlate with cadaveric literature, there is no guarantee the resulting kinematics represent subject-specific TFJ and PFJ kinematics.

The framework developed in this study represents a significant contribution to the field of personalised musculoskeletal modelling. This was the first study which used the MAP-Client framework for the development of personalised models and assessed their suitability for subsequent musculoskeletal simulations. In addition to using the framework, a number of improvements and additions were made using the MAP-Client architecture. Most prominently, the definition of MTU intermediate pathways. In addition to overcoming issues in the current MAP-Client framework, the proposed framework overcomes issues relating to the current personalised modelling methods. Several processes which have previously been completed manually, are automated within this framework, reducing the time demands and subjectivity associated with generating these personalised models. These primarily related to numerous errors which can occur in both scaled and personalised models. These errors were first defined conceptually, and then mathematically which allowed for the automatic detection and fixing of these errors. Future work may focus on improving the MTU intermediate pathway definitions and optimisation as well as the development of personalised TFJ and PFJ kinematic models which do not compromise MTU kinematics.

**Declarations**

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**Conflicts of interest**

The authors declare no conflict of interest relating to the presented work.
Availability of data and material

The models generated as part of this research are available upon reasonable request from the corresponding author.

Code availability

The pre-existing MAP-Client is freely available here: https://map-client.readthedocs.io/en/latest/ with additional information provided here https://simtk.org/projects/map. The developed frame generated as part of this research are available upon reasonable request from the corresponding author.
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OpenSim models on lower-body kinematics and knee ligament lengths. Journal of Biomechanics 83:9-15


Figure 4
Figure 5
Figure 7
Figure 8
Figure 9
**Fig 1:** Schematic representation of the computational workflow used within this study. Detailed is each of the development steps implemented and the indication of each model’s position within the development workflow.

**Fig 2:** Right leg sartorius MTU kinematic curves for participant M02 where left plot is MTU length and right plot is TFJ flexion moment arm. Black lines are for the linearly scaled gait2392 model, green lines are combined cadaveric literature data, red lines represent Model 2, and blue lines represent Model 4.

**Fig 3:** Right leg semimembranosus MTU kinematic curves for participant M03 where left plot is MTU length and right plot is TFJ flexion moment arm. Black lines are for the linearly scaled gait2392 model, green lines are combined cadaveric literature data, red lines represent Model 2, and blue lines represent Model 4.

**Fig 4:** Left leg sartorius MTU kinematic curves for participant M01 where left plot is MTU length and right plot is TFJ flexion moment arm. Black lines are for the linearly scaled gait2392 model, green lines are combined cadaveric literature data, red lines represent Model 4, and blue lines represent Model 5.

**Fig 5:** Right leg rectus femoris MTU kinematic curves for participant M01 where left plot is MTU length and right plot is TFJ flexion moment arm. Black lines are for the linearly scaled gait2392 model, green lines are combined cadaveric literature data, red lines represent Model 4, and blue lines represent Model 5.

**Fig 6:** Right tibiofemoral joint of the (A) generic gait2392 model and (B) MAP-Client generated model at 100° of tibiofemoral joint flexion. Note the higher amount of tibial superior translation in (B) the MAP-Client generated model, which acts to increase the gastrocnemii MTU lengths with increasing flexion, hence appearing to be an extensor.

**Fig 7:** Tibiofemoral joint motion from standard MAP-Client generated models for each participant and each of the 6 DOFs where each colour represents a different participant. Translations are reported in metres and rotations in radians. Note that each motion is expressed relative to the TFJ flexion angle.
**Fig 8:** Personalised TFJ kinematics for each participant and each of the 6 DOFs where each colour represents a different participant. Translations are reported in metres and rotations in radians. Note that each motion is expressed relative to the TFJ flexion angle.

**Fig 9:** Personalised PFJ motion for each participant and each of the 6 DOFs where each colour represents a different participant. Translations are reported in metres and rotations in radians. Note that each motion is expressed relative to the TFJ flexion angle.
**Table 1:** Demographic data pertaining to study participants.

<table>
<thead>
<tr>
<th>Participant</th>
<th>Gender</th>
<th>Limb</th>
<th>Age (years)</th>
<th>Height (cm)</th>
<th>Weight (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>M01</td>
<td>M</td>
<td>R</td>
<td>24</td>
<td>182.0</td>
<td>82</td>
</tr>
<tr>
<td>M02</td>
<td>F</td>
<td>R</td>
<td>22</td>
<td>172.0</td>
<td>63</td>
</tr>
<tr>
<td>M03</td>
<td>M</td>
<td>R</td>
<td>23</td>
<td>180.0</td>
<td>88</td>
</tr>
<tr>
<td>M07</td>
<td>M</td>
<td>L</td>
<td>32</td>
<td>185.0</td>
<td>89</td>
</tr>
<tr>
<td>M09</td>
<td>M</td>
<td>L</td>
<td>31</td>
<td>161.0</td>
<td>45</td>
</tr>
<tr>
<td>M11</td>
<td>F</td>
<td>L</td>
<td>21</td>
<td>160.5</td>
<td>55</td>
</tr>
</tbody>
</table>

(n or means±sd) 4M & 2F  3L & 3R  25.5±4.8  173.4±10.7  70.3±18.6

M-males, F-females; L-left, R-right; sd-standard deviation
Table 2: Explanations of each of the 5 models developed as part of this study.

<table>
<thead>
<tr>
<th>Model</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Model 1</td>
<td>Linear scaled gait (Delp et al. 2007) model</td>
</tr>
<tr>
<td>Model 2</td>
<td>Standard MAP-Client model where via points were replaced with wrapping surfaces</td>
</tr>
<tr>
<td>Model 3</td>
<td>Model 2 with personalised TFJ and PFJ mechanisms</td>
</tr>
<tr>
<td>Model 4</td>
<td>Model 2 following MTU wrapping-surface optimisation</td>
</tr>
<tr>
<td>Model 5</td>
<td>Model 3 following MTU wrapping-surface optimisation</td>
</tr>
</tbody>
</table>
**Table 3.** Summary comparison between MAP-Client model with fitted wrapping surfaces (Model 2) and MAP-Client model with optimised wrapping surfaces (Model 4). Displayed is the number of occurrences, for each MTU group and all combined MTUs, where the metric was either (+) improved, (-) worse, or (±) no change. For each MTU group, sample size was 48 (8 MTUs x 6 subjects). For all combined MTUs, sample size was 144 (8 per group x 3 groups x 6 subjects). Statistically significant differences are denoted using coloured cells, where yellow indicates no change, green indicates improvement, and red indicates worsening. In cases of no statistically significant difference between either of the three options, cells were left unshaded.

<table>
<thead>
<tr>
<th>Metric</th>
<th>Polarity penalty</th>
<th>Muscle penetration</th>
<th>Length smoothness</th>
<th>Moment arm smoothness</th>
<th>Moment arm gradient</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>+</td>
<td>-</td>
<td>±</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td><strong>All MTUs</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Polarity penalty</td>
<td>23, 5</td>
<td>116</td>
<td>48, 3</td>
<td>93</td>
<td>28, 9</td>
</tr>
<tr>
<td>Muscle penetration</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Polarity penalty</td>
<td>0, 0</td>
<td>48</td>
<td>5, 2</td>
<td>41</td>
<td>13, 0</td>
</tr>
<tr>
<td>Muscle penetration</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Length smoothness</td>
<td>9, 4</td>
<td>35</td>
<td>16, 1</td>
<td>31</td>
<td>9, 4</td>
</tr>
<tr>
<td>Moment arm smoothness</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Moment arm smoothness</td>
<td>14, 1</td>
<td>33</td>
<td>27, 0</td>
<td>21</td>
<td>6, 5</td>
</tr>
<tr>
<td>Moment arm gradient</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Where + represents improvement from model 2 to model 4, - represents worsening from model 2 to model 4, and ± represents no change between models 2 and 4.
Table 4. Summary comparison between MAP-Client model with fitted wrapping surfaces and joint mechanisms (Model 3) and MAP-Client model with optimised wrapping surfaces and joint mechanisms (Model 5). Displayed is the number of occurrences, for each MTU group and all combined MTUs, where the metric was either (+) improved, (-) worse, or (±) no change. For each MTU group, sample size was 48 (8 MTUs x 6 subjects). For all combined MTUs, sample size was 144 (8 per group x 3 groups x 6 subjects). Statistically significant differences are denoted using coloured cells, where yellow indicates no change, green indicates improvement, and red indicates worsening. In cases of no statistically significant difference between either of the three options, cells were left unshaded.

<table>
<thead>
<tr>
<th>Polarity penalty</th>
<th>Muscle penetration</th>
<th>Length smoothness</th>
<th>Moment arm smoothness</th>
<th>Moment arm gradient</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>-</td>
<td>±</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>All MTUs</td>
<td>25, 4, 2.8%</td>
<td>115, 45, 10, 89, 26, 18, 100, 71, 29, 44, 135, 9, 0, 17.4%</td>
<td>79.9%, 31.3%, 6.9%, 61.8%, 18.1%, 12.5%, 69.4%, 49.3%, 20.1%, 30.6%, 93.8%, 6.3%, 0%</td>
<td></td>
</tr>
<tr>
<td>Quadriceps MTU group</td>
<td>1, 1, 46, 9, 4, 35, 6, 7, 35, 21, 9, 18, 46, 2, 0, 2.1%</td>
<td>95.8%, 18.8%, 8.3%, 72.9%, 12.5%, 14.6%, 72.9%, 43.8%, 18.8%, 37.5%, 95.8%, 4.2%, 0%</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hamstrings MTU group</td>
<td>12, 25%, 2, 4.2%, 34, 15, 1, 32, 7, 7, 34, 21, 11, 16, 43, 5, 0, 70.8%, 31.3%, 2.1%, 66.7%, 14.6%, 14.6%, 70.8%, 43.8%, 22.9%, 33.3%, 89.6%, 10.4%, 0%</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Extras MTU group</td>
<td>12, 25%, 1, 2.1%, 35, 21, 5, 22, 13, 4, 31, 29, 9, 10, 46, 2, 0, 72.9%, 43.8%, 10.4%, 45.8%, 27.1%, 8.3%, 64.6%, 60.4%, 18.8%, 20.8%, 95.8%, 4.2%, 0%</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Where + represents improvement from model 3 to model 5, - represents worsening from model 3 to model 5, and ± represents no change between models 3 and 5.
Table 5. Summary comparison between MAP-Client model with optimised wrapping surfaces (Model 4) and MAP-Client model with optimised wrapping surfaces and TFJ-PFJ mechanism (Model 5). Displayed is the number of occurrences, for each MTU group and all combined MTUs, where the metric was either (+) improved, (-) worse, or (±) no change. For each MTU group, sample size was 48 (8 MTUs x 6 subjects). For all combined MTUs, sample size was 144 (8 per group x 3 groups x 6 subjects). Statistically significant differences are denoted using coloured cells, where yellow indicates no change, green indicates improvement, and red indicates worsening. In cases of no statistically significant difference between either of the three options, cells were left unshaded.

<table>
<thead>
<tr>
<th>Polarity penalty</th>
<th>Muscle penetration</th>
<th>Length smoothness</th>
<th>Moment arm smoothness</th>
<th>Moment arm gradient</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>-</td>
<td>±</td>
<td>+</td>
<td>-</td>
</tr>
<tr>
<td>27, 13, 104, 3, 25, 116, 20, 27, 97, 43, 48, 53, 66, 78, 0, 18.8% 9% 72.7% 2.1% 17.4% 80.6% 13.9% 18.8% 67.4% 29.9% 33.3% 36.8% 45.8% 54.2% 0%</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>All MTUs</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0, 1, 47, 0, 11, 37, 3, 16, 29, 14, 16, 18, 24, 24, 0, 0% 2.1% 97.9% 0% 22.9% 77.1% 6.3% 33.3% 60.4% 29.2% 33.3% 37.5% 50% 50% 0%</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Quadriceps MTU group</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>6, 4, 38, 2, 4, 42, 6, 6, 36, 15, 15, 18, 19, 29, 0, 12.5% 8.3% 79.2% 4.2% 8.3% 87.5% 12.5% 12.5% 75% 31.3% 31.3% 37.5% 39.6% 60.4% 0%</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Hamstrings MTU group</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>21, 8, 19, 1, 10, 37, 11, 5, 32, 14, 17, 17, 23, 25, 0, 43.8% 16.7% 39.6% 2.1% 20.8% 77.1% 22.9% 10.4% 66.7% 29.2% 35.4% 35.4% 47.9% 52.1% 0%</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Extras MTU group</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Where + represents improvement from model 4 to model 5, - represents worsening from model 4 to model 5, and ± represents no change between models 4 and 5.
Table 6. Performance criteria results for the MAP-Client model with optimised wrapping surfaces and a generic joint model (Model 4).

<table>
<thead>
<tr>
<th></th>
<th>Polarity penalty</th>
<th>Muscle penetration</th>
<th>Length smoothness</th>
<th>Moment arm smoothness</th>
<th>Moment arm gradient error</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>M01</strong></td>
<td>7 (29.2%)</td>
<td>0 (0.0%)</td>
<td>1.06 ± 0.2</td>
<td>1.36 ± 0.9</td>
<td>97.88 ± 251.9</td>
</tr>
<tr>
<td><strong>M02</strong></td>
<td>7 (29.2%)</td>
<td>0 (0.0%)</td>
<td>1.37 ± 1.3</td>
<td>1.36 ± 0.8</td>
<td>36.46 ± 49.7</td>
</tr>
<tr>
<td><strong>M03</strong></td>
<td>5 (20.84%)</td>
<td>1 (4.2%)</td>
<td>1.23 ± 0.7</td>
<td>1.32 ± 0.4</td>
<td>87.62 ± 151.3</td>
</tr>
<tr>
<td><strong>M07</strong></td>
<td>7 (29.2%)</td>
<td>4 (16.7%)</td>
<td>1.17 ± 0.2</td>
<td>1.40 ± 0.6</td>
<td>110.94 ± 188.7</td>
</tr>
<tr>
<td><strong>M09</strong></td>
<td>6 (25.0%)</td>
<td>2 (8.3%)</td>
<td>1.06 ± 0.2</td>
<td>1.30 ± 0.6</td>
<td>54.42 ± 87.3</td>
</tr>
<tr>
<td><strong>M11</strong></td>
<td>5 (20.8%)</td>
<td>1 (4.2%)</td>
<td>1.13 ± 0.2</td>
<td>1.72 ± 0.6</td>
<td>142.36 ± 186.1</td>
</tr>
</tbody>
</table>

Where polarity penalty and muscle penetration are reported as the number and percentage of occurrences of each penalty, and the remaining metrics are reported as the average ± standard deviation across each of the 24 muscles considered in this analysis. In all cases, a lower value represents a better result.
Table 7. Performance criteria results for the MAP-Client model with optimised wrapping surfaces and a personalised joint model (Model 5).

<table>
<thead>
<tr>
<th></th>
<th>Polarity penalty</th>
<th>Muscle penetration</th>
<th>Length smoothness</th>
<th>Moment arm smoothness</th>
<th>Moment arm gradient error</th>
</tr>
</thead>
<tbody>
<tr>
<td>M01</td>
<td>3 (12.5%)</td>
<td>3 (12.5%)</td>
<td>1.41 ± 0.9</td>
<td>1.46 ± 0.7</td>
<td>422.44 ± 1126.1</td>
</tr>
<tr>
<td>M02</td>
<td>0 (0.0%)</td>
<td>2 (8.3%)</td>
<td>0.99 ± 0.2</td>
<td>1.33 ± 0.4</td>
<td>32.50 ± 35.6</td>
</tr>
<tr>
<td>M03</td>
<td>4 (16.7%)</td>
<td>5 (20.8%)</td>
<td>1.58 ± 2.1</td>
<td>1.83 ± 1.9</td>
<td>438.29 ± 1983.8</td>
</tr>
<tr>
<td>M07</td>
<td>4 (16.7%)</td>
<td>9 (37.5%)</td>
<td>1.62 ± 1.6</td>
<td>1.71 ± 0.9</td>
<td>150.03 ± 302.1</td>
</tr>
<tr>
<td>M09</td>
<td>5 (20.8%)</td>
<td>5 (20.8%)</td>
<td>1.32 ± 0.2</td>
<td>1.29 ± 0.4</td>
<td>169.25 ± 321.1</td>
</tr>
<tr>
<td>M11</td>
<td>4 (16.7%)</td>
<td>6 (25.0%)</td>
<td>1.14 ± 0.2</td>
<td>1.68 ± 1.1</td>
<td>186.06 ± 353.7</td>
</tr>
</tbody>
</table>

Where polarity penalty and muscle penetration are reported as the number and percentage of occurrences of each penalty, and the remaining metrics are reported as the average ± standard deviation across each of the 24 muscles considered in this analysis. In all cases, a lower value represents a better result.
Appendix 1: Common non-physiological MTU kinematics and non-physical MTU pathways

Within a majority of generic OpenSim models, MTU intermediate pathways are predominantly defined using a combination of fixed and conditional via points. The use of via points allows users to define highly constrained MTU pathways. While this approach works in generic linear scaled models, transferring these via points to personalised models is a non-trivial task. Previous studies (Modenese et al. 2018; Scheys et al. 2006), as well as the MAP-Client have used non-rigid morphing methods to fit these via points to personalised bone geometries. While these methods work in theory, within the MAP-Client, they often introduce non-physical pathways (Figure S1) and non-physiological MTU kinematics (Figure S2). Non-physical pathways refer to pathways which contain 90° turns and penetrate bone surfaces. Non-physiological MTU kinematics refer to MTU lengths which are not continuous and contain discontinuities or do not follow the patterns (represented as the change in moment arm magnitude with respect to joint angle) of previously published cadaveric literature data.

Figure 10: Examples of (A, B, C) non-physiological MTU shapes and (C, D, E, F) MTU bone penetration in a standard MAP-Client generated model with morphed via points.
Figure 11: The MTU lengths and moment arms from a standard MAP-Client generated model (red), generic gait2392 model (black), and cadaveric literature data (green) for the rectus femoris, medial gastrocnemius, and vastus lateralis where discontinuities are highlighted in black boxes.
Appendix 2: Detailed optimisation and evaluation criteria

The optimisation method was written using open-source Python packages and deployed on the Griffith University High Performance Computing Cluster “Gowonda” (https://conf- ers.griffith.edu.au/display/GHCD/Gowonda+HPC) enabling parallelisation. The optimisation method used within this framework is referred to as particle swarm optimisation (PSO) (pyswarm: A Python package for particle swarm optimization (PSO) with constraint support, Abraham D. Lee, https://pythonhosted.org/pyswarm/). PSO simultaneously searches different regions of the solution space using different “particles”. During each iteration, MTU length and moment arms were calculated and tested against various objective criteria and penalty functions.

MTU moment arms calculated using OpenSim are highly sensitive to small changes in MTU length. To overcome this and increase computational speed, previously published methods for accurate estimations of MTU moment arms were implemented. This implementation uses cubic B-splines fit to MTU lengths across the TFJ flexion/extension range of motion (Sartori et al., 2012). MTU moment arms are then calculated as the partial derivatives of these splines, i.e., changes in length divided by changes in joint angle. To ensure this process was not artificially increasing the calculated MTU length smoothness (covered below), the normalised error (splineNormErr) between the OpenSim calculated and cubic B-splined MTU lengths was calculated and minimised within the optimisation framework.

Patterns of MTU kinematics were represented as gradients with respect to joint angle (change in MTU moment arm/length divided by the change in joint angle), therefore pattern similarity was assessed using the normalised error between the gradients (maGradErr) of the modelled (MAP-Client personalised model) and target data (cadaveric literature data). Further objective functions were created to measure and control curve smoothness to ensure smooth and continuous MTU kinematics. The smoothness measure relied on three assumptions. First, MTU kinematic curves were primarily monophasic with no significant peaks or troughs, which is correct when the joints are moved through physiological ranges. Second, the gradient of the curves was constant with respect to MTU length or slowly changing in the case of MTU moment arms. The third and final assumption was that if MTU kinematic curves were a perfectly straight line, the second derivative of this line would be zero. As a consequence, if the MTU kinematics had only slightly changing gradients the second derivative would approximate zero. Therefore, kinematic smoothness was defined as the number of modelled curve (MAP-Client personalised model) derivatives required for the differentiated curve’s
range, mean, and maximum to fall below predefined thresholds. The smoothness measure of
the tested curve was then normalised to the smoothness measure of the target data. It should be
noted that only the generic OpenSim model data were used to normalise the smoothness
measure whereby the average smoothness measure of the two generic OpenSim models (see
below) was used. As mentioned above, the objective criteria used a number of targets within
the optimisation.

Target data were taken from multiple sources, but can be divided into two distinct categories:
model data and literature data. Model data were obtained from two generic OpenSim models,
the gait2392 model (Delp et al., 2007), on which MAP-Client models are based, and the more
recent Fullbody Model (Rajagopal et al., 2016). Unlike model data, literature data were taken
from a wide range of different studies carried out on cadavers (Arnold et al., 2010; Buford et
al., 1997; Draganich et al., 1987; Fick, 1879; Navacchia et al., 2017; Pal et al., 2007; Spoor
and van Leeuwen, 1992; Visser et al., 1990; Wilson and Sheehan, 2009). These values were
combined for each MTU, and the mean and standard deviation calculated.

Optimisation criteria and penalty functions were employed to mathematically detect various
errors commonly observed in MTU kinematics and pathways.

Each MTU’s moment arm was required to have a mechanical action about a joint DOF (e.g.
flexion or extension) consistent with target data (Figure S3). This was termed “polarity of the
moment arm” and a penalty was defined to ensure these were physiological (moment arm
polarity penalty). At each TFJ flexion angle, the polarity of the tested model (i.e., MAP-Client
personalised model) and the generic gait2392 model was compared. If the polarity was the
same, no penalty was applied, else a secondary test was performed. Specifically, the adjacent
20 angles (i.e., ±10°) were checked. If the polarity of the tested model within this range matched
the target data, the discrepancy was no longer considered a polarity error. When this condition
was not met, a penalty was applied to the final weighted value.
Figure 12: Example of MTU moment arm polarity error in the MAP-Client generated model (red) compared to both generic model (black) and literature (green) data. Depending on where a MTU intersects an associated wrapping cylinder, it may wrap entirely around it, i.e., complete a full circumferential loop before continuing to the insertion point (Figure S4A). To avoid these non-physical MTU pathways, the MTU path points in the neutral position were queried. These points represent the origin, insertion, and via points as well as the points where the MTU starts and finishes wrapping (Figure S4B). With the assumption that each MTU path point is inferior compared to the previous path point (which is true in the neutral position), the superior/inferior coordinate of each path point is tested. If the superior/inferior coordinate of a path point was greater than the superior/inferior coordinate of the previous path point this was indicative of a wrapping error.

Figure 13: (A) Example of MTU wrapping error in an OpenSim model whereby the MTU wraps around the circumference of the cylinder and (B) associated MTU path points numbered sequentially where points 3 and 4 illustrate the wrap error.

MTU bone penetration penalty employed an automated detection algorithm. Initially, the joints that each MTU spanned and the bodies (i.e., bones) they could penetrate were determined. Similar to the wrap error penalty, each MTU path point is determined and a vector calculated between adjacent path points. Due to limitation in the OpenSim application programming
interface (API), the path between wrap on/off points cannot be readily determined. As a result the penalty only considered vectors that intersected bone surfaces between either: (i) two fixed points (e.g., origin or via point), (ii) a fixed point and a wrapping on point, (iii) a wrapping off and wrapping on point (on different wrapping surfaces), and (iv) a wrapping off point and a fixed point (Figure S5). It was assumed that if the on/off wrapping points did not penetrate, the intermediate path also did not penetrate.

![Diagram](image)

**Figure 14:** (A) Illustration of the vastus medialis pathway at 100° of TFJ flexion within OpenSim and (B) each of the path points available within the OpenSim API. Where points 1, 6, 7, and 8 are fixed points, points 2 and 4 are wrapping on points, and points 3 and 5 are wrapping off points. Using the proposed framework, tested path point pairs are: 1-2, 3-4, 5-6, 6-7, and 7-8.

Once each of the penalties had been determined, they were combined into a single penalty value where each penalty function, if returning a positive test, attracted penalty value. The aforementioned penalty functions and objective criteria were combined into a single weighted value, which was minimised via optimisation (Equation 1).

\[
\text{wv} = \text{splineLenN} + \text{lenN} + \text{splineNormErr} + \text{maGradErr} + \text{pen}
\]

where, \(wv\), is the weighted value, \(\text{splineLenN}\), is the smoothness measure of the splined lengths fit to the OpenSim MTU lengths, \(\text{lenN}\), is the smoothness measure of the OpenSim API derived MTU lengths, \(\text{splineNormErr}\), is the normalised error between the OpenSim derived and cubic B-spline fit MTU lengths, \(\text{maGradErr}\), is the normalised error between the MTU moment arms and target data, and, \(\text{pen}\), is the summed penalty value.
### Appendix 3: Model evaluation criteria results for Models 1, 2, and 3

#### Table 8: Performance criteria results for linear scaled gait2392 model (Model 1).

<table>
<thead>
<tr>
<th></th>
<th>Polarity penalty</th>
<th>Muscle penetration</th>
<th>Length smoothness</th>
<th>Moment arm smoothness</th>
<th>Moment arm gradient error</th>
</tr>
</thead>
<tbody>
<tr>
<td>M01</td>
<td>0 (0%)</td>
<td>0 (0%)</td>
<td>1.02 ± 0.1</td>
<td>1.24 ± 0.2</td>
<td>464.2 ± 448.2</td>
</tr>
<tr>
<td>M02</td>
<td>0 (0%)</td>
<td>0 (0%)</td>
<td>1.02 ± 0.1</td>
<td>1.24 ± 0.2</td>
<td>520.9 ± 538.67</td>
</tr>
<tr>
<td>M03</td>
<td>0 (0%)</td>
<td>0 (0%)</td>
<td>1.02 ± 0.2</td>
<td>1.26 ± 0.2</td>
<td>465.8 ± 458.4</td>
</tr>
<tr>
<td>M07</td>
<td>0 (0%)</td>
<td>0 (0%)</td>
<td>1.06 ± 0.2</td>
<td>1.22 ± 0.2</td>
<td>457.7 ± 451.1</td>
</tr>
<tr>
<td>M09</td>
<td>0 (0%)</td>
<td>0 (0%)</td>
<td>1.06 ± 0.1</td>
<td>1.20 ± 0.2</td>
<td>459.7 ± 441.4</td>
</tr>
<tr>
<td>M11</td>
<td>0 (0%)</td>
<td>0 (0%)</td>
<td>1.02 ± 0.1</td>
<td>1.24 ± 0.2</td>
<td>465.1 ± 542.8</td>
</tr>
</tbody>
</table>

Where polarity penalty and muscle penetration are reported as the number and percentage of occurrences of each penalty, and the remaining metrics are reported as the average ± standard deviation across each of the 24 muscles considered in this analysis. In all cases, a lower value represents a better result.

#### Table 9: Performance criteria results for the MAP-Client model with fit wrapping surfaces and a generic joint model (Model 2).

<table>
<thead>
<tr>
<th></th>
<th>Polarity penalty</th>
<th>Muscle penetration</th>
<th>Length smoothness</th>
<th>Moment arm smoothness</th>
<th>Moment arm gradient error</th>
</tr>
</thead>
<tbody>
<tr>
<td>M01</td>
<td>7 (29.2%)</td>
<td>8 (33.3%)</td>
<td>3.5 ± 11.5</td>
<td>1.5 ± 0.4</td>
<td>1270.8 ±1964.14</td>
</tr>
<tr>
<td>M02</td>
<td>4 (16.7%)</td>
<td>8 (33.3%)</td>
<td>1.1 ± 0.2</td>
<td>3.1 ± 6.5</td>
<td>19527 ± 72014</td>
</tr>
<tr>
<td>M03</td>
<td>7 (29.2%)</td>
<td>8 (33.3%)</td>
<td>1.4 ± 1.1</td>
<td>1.6 ± 1.1</td>
<td>1891.7 ±4145.5</td>
</tr>
<tr>
<td>M07</td>
<td>6 (25.0%)</td>
<td>9 (37.5%)</td>
<td>1.3 ± 0.8</td>
<td>1.42 ± 0.9</td>
<td>1704.2 ±2666.1</td>
</tr>
<tr>
<td>M09</td>
<td>5 (20.8%)</td>
<td>13 (54.2%)</td>
<td>2.1 ± 4.8</td>
<td>6.7 ± 20.6</td>
<td>55325.7 ± 182702</td>
</tr>
<tr>
<td>M11</td>
<td>8 (33.3%)</td>
<td>7 (29.2%)</td>
<td>3.4 ± 10.8</td>
<td>6.8 ± 23.4</td>
<td>42438.2 ±20233</td>
</tr>
</tbody>
</table>

Where polarity penalty and muscle penetration are reported as the number and percentage of occurrences of each penalty, and the remaining metrics are reported as the average ± standard deviation across each of the 24 muscles considered in this analysis. In all cases, a lower value represents a better result.
Table 10: Performance criteria results for the MAP-Client model with fit wrapping surfaces and a personalised joint model (Model 3).

<table>
<thead>
<tr>
<th></th>
<th>Polarity penalty</th>
<th>Muscle penetration</th>
<th>Length smoothness</th>
<th>Moment arm smoothness</th>
<th>Moment arm gradient error</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>M01</strong></td>
<td>10 (41.7%)</td>
<td>8 (33.3%)</td>
<td>2.7 ± 7.6</td>
<td>2.8 ± 5.3</td>
<td>9915.8 ± 416417.7</td>
</tr>
<tr>
<td><strong>M02</strong></td>
<td>4 (16.7%)</td>
<td>12 (50%)</td>
<td>1.6 ± 2.1</td>
<td>5.7 ± 18</td>
<td>33246.5 ± 157718</td>
</tr>
<tr>
<td><strong>M03</strong></td>
<td>3 (12.5%)</td>
<td>10 (41.7%)</td>
<td>1.2 ± 0.2</td>
<td>1.5 ± 0.5</td>
<td>683.9 ± 741.9</td>
</tr>
<tr>
<td><strong>M07</strong></td>
<td>6 (25%)</td>
<td>9 (37.5%)</td>
<td>1.1 ± 0.2</td>
<td>3.7 ± 5.5</td>
<td>7808.9 ± 13452.1</td>
</tr>
<tr>
<td><strong>M09</strong></td>
<td>12 (50%)</td>
<td>15 (60%)</td>
<td>1.7 ± 1.8</td>
<td>7.2 ± 17.3</td>
<td>45440.5 ± 147443</td>
</tr>
<tr>
<td><strong>M11</strong></td>
<td>9 (37.5%)</td>
<td>11 (45.8%)</td>
<td>1.12 ± 0.19</td>
<td>3.9 ± 9.7</td>
<td>22362.5 ± 96077.7</td>
</tr>
</tbody>
</table>

Where polarity penalty and muscle penetration are reported as the number and percentage of occurrences of each penalty, and the remaining metrics are reported as the average ± standard deviation across each of the 24 muscles considered in this analysis. In all cases, a lower value represents a better result.