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Analyzing ligament prestrain in a multibody model of an ankle joint with random sampling

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1. Introduction

The joints of the lower limb are the key elements in enabling the interaction of the body and the ground during gait [2]. At the same time, the ankle represents one the first links in this load-transferring mechanism. The problems and applications of digital twin modeling, which represent highly accurate and validated models used for treatment and surgical planning, are becoming ever more popular as indicated by recent publications [15], [16]. Nevertheless, these models require modern and advanced tools for validation and efficient exploration of the solution space. This is only even more evidenced by the complex nature of the body joints present in the lower limb.

The ankle joint, analyzed in this study, contains multiple subjoints, which form an intricate structure with three-dimensional articulation. This paper focuses on the part of the ankle sometimes referred to as the true ankle joint, in which the talus and tibia are connected. This subjoint is mostly responsible for plantar- and dorsiflexion, which can be seen as flexion and extension in the sagittal plane of the lower limb. The joint connects the aforementioned bones through a layer of cartilage and a complex system of ligaments. The ligaments resemble nonlinear cables in their function, while the articular surfaces could be seen as deformable contact pairs, transferring mostly compressive loads.

Two main approaches for modeling this structure can be observed in the literature. The first one employs the Finite Element Method (FEM), which makes it possible to accurately represent the load distribution in structures with complex geometry [9], including modeling implants and more [21], albeit at a high numerical cost. The method is very useful in analyzing biomechanical models, however, its applications are still somewhat limited due to available computing power, especially in problems regarding dynamics, optimization and uncertainty quantification. That is why, the models formulated under the Multibody System (MBS) framework are very common [22], [23]. It is worth mentioning that in many cases the models obtained with FEM and MBS differ mostly in the description of contact in the articular surfaces. FEM offers a much more viable option in this case, while MBS provides a rough, but fast approximation. Interestingly, in case of MBS method many distinct subapproaches to modeling can be observed. In some models, the articular surfaces are treated as rigid and modeled with constraint equations [6]. Other models treat all of the elements of the ankle as deformable [1], [4]. The ankle can also be replaced with kinematic pairs typically found in mechanism and machine theory [14], [17]. Other methods to assess contact biomechanics were also tested for different joints [18], [19]. Finally, the models can also be subdivided into two-dimensional [1] and three-dimensional [14].

Regardless of the assumed modeling method, it is typical to model the ligaments in the joint with nonlinear cables [1], [10], [22], [23]. This representation captures the essential characteristics of these elements, while being numerically efficient.

Modeling such an intricate, nonlinear system is a difficult task, which is only compounded by the fact that typical body joints function in a state of prestrain [11]. The prestrain considered in this study can be defined as a complex phenomenon, in which certain elements of the joint are under strain, even when no external load is applied to it. In biomechanical models of the ankle, or other synovial joints, such as the knee, the prestrain is usually applied to the ligaments. Its implementation is rather simple as it only requires setting the initial length of the cable, also refereed to as slack or free length, to a proper value. While the implementation might be simple, choosing the proper value for the slack length is a very complicated problem. Medical scans, used for generating patient-specific data, do not provide any information on the internal state of the joint. Therefore, the slack length value is typically obtained through invasive experiments [13], which require the ligament to be excised from the joint. Such an approach does not complement the digital twin trend, popular in biomechanics. Even if the experiment was noninvasive, the uncertainty in measurement of slack length could create many problems as the typical prestrain values are very low, often close to 2 %.

In the literature, three main approaches could be found to address the problem of obtaining slack lengths in a numerical way. The simplest one is to choose a strain-free configuration for the joint, often corresponding to its rest configuration. The lengths of the ligaments computed in this configuration serve as the slack lengths for the subsequent simulations. In this approach the ligament prestrain is effectively omitted. The second option is to apply low, arbitrary prestrain values to the ligaments. This is typically done by shortening the ligament lengths obtained in the reference configuration by 2 % [3], [8], [10], [22], [23]. The trend seems to be dominant in the ankle joint modeling. However, the arbitrary shortening often results in the change of the equilibrium of the model, impacting its output characteristics, such as angular displacement. The next possibility is to shorten the ligaments based on the actual experimental results published in the literature [5]. Although this seems like the most attractive option, it should be mentioned that slack lengths are patient-specific, linked to joint geometry and material properties. When such specific experimental values are applied to an arbitrary joint model, they might result in unbalanced load system, as seen in [5]. Finally, it should be mentioned that slack lengths can also be optimized along other model parameters, in order to fit the model to a desired reference characteristic [6]. This however, requires reference joint characteristics, which are not always available, especially for problems regarding digital twin modeling. Furthermore, during optimization, the ligaments along with their slack lengths might lose their original function, making it difficult to ascertain the true impact of prestrain.

In [5], it was shown that the currently available modeling approaches to ligament prestrain only approximate the real phenomenon, while also significantly affecting the results obtained from the model. It remains unclear, which of the approaches offers the results closest to reality. A potential solution to the problem is to compare the methods on a large collection of models with established reference characteristics. However, this would be a significant undertaking and would not directly apply to new or untested digital twin models without known reference outputs. Additionally, due to low physical levels of prestrain, potential uncertainties in measurement could make the analysis more difficult.

On the other hand, while shortening slack lengths alters the model in an unpredictable manner [5], the resulting model is still a prestrained variant of the original. Even through it differs from the original, it shares similarities with it in terms of parameters and output, and, more importantly, it can be seen as the much needed reference, but obtained in a numerical way. The main idea of this study is take advantage of this property and generate multiple random prestrained models resembling the original. Then, test and compare the prestrain approaches on the generated models.

2. Method

The main objective of the approach was to use an existing ankle model to generate a large number of its random prestrained variants. These models would form a reference dataset to analyze common prestrain approaches. In the first part of this section, the assumed model of the ankle joint is introduced. The second section focuses on the details regarding the prestrain approaches employed in the study, while the third one describes the procedure used to generate and prestrain the random variants of the base model.

2.1. The assumed model of the ankle joint

The base model of true ankle joint used in this study was assumed after [1]. It contains six nonlinear cables, which model the ligaments, and two contact pairs that deform to represent the articular surfaces of the ankle joint, see Fig. 1.

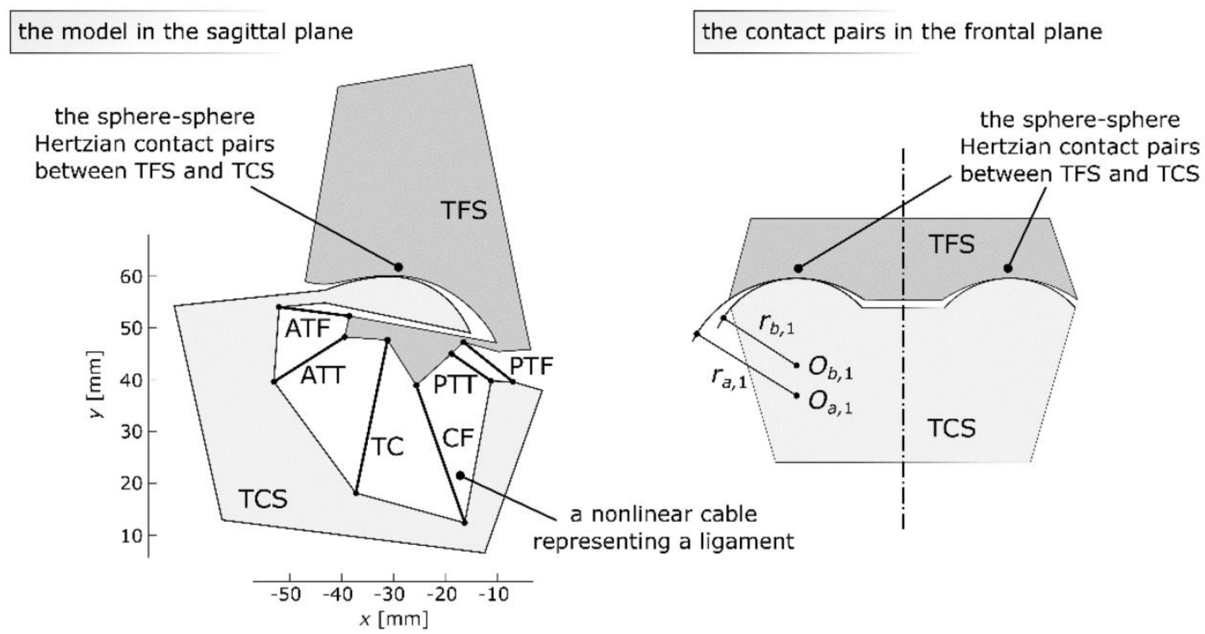

Fig 1. The model of the ankle joint analyzed in this study. Reproduced with permission from [1].

The ligaments considered in this model are: the anterior tibiotalar ligament (ATT), tibiocalcaneal ligament (TC), posterior tibiotalar ligament (PTT), anterior talofibular ligament (ATF), calcaneofibular ligament (CF), and posterior talofibular ligament (PTF). Their force values can be obtained from an an exponential, assumed after [7]:

$$F_i = A_i \left(exp\left(B_i \frac{l_{cur,i} - l_{slack,i}}{l_{slack,i}} \right) - 1 \right) \qquad (1)$$

where: F_i – the force generated by the cable when its elongated; A_i/B_i – the material parameters for the ligament model, $l_{cur,i}$ – the current length of the cable for the given configuration, $l_{slack,i}$ – the slack length of the cable (often referred to as free or initial length).

The contact pairs were modeled as Hertzian of sphere-sphere type, as in [1], [12], while the model was loaded with an external moment of -5 Nm to 5 Nm in 51 steps. The system was defined by two governing equations. The first one, representing for force equilibrium, contained the sum of the forces generated by the ligaments and the contact pairs. The second one, for moment equilibrium, consisted of the sum of the moments from the ligaments and contact pairs as well as the external flexion moment acting on the system. The solutions, in the form of model configuration, were obtained with Levenberg–Marquardt method implemented in *Scipy* [20]. The obtained solution was accepted if the sum of the residual loads (F_x, F_y and M) was less than $1.0\times10-8$.

The main output of the model, i.e. the angular stiffness, was obtained by computing the angular displacement under external moment loads with reference to the equilibrium configuration.

2.2. Including prestrain in the model

The prestrain can be included in the model simply by modifying the slack lengths in the force equation for the cables representing ligaments. Two major approaches to the computation of slack lengths can be found in the literature. The first one, referred to as strain-free in this study, assumes that these lengths are equal to lengths of the links in the rest configuration of the model. This makes the solution elegant and simply, but effectively omits prestrain, as by definition assumes a strain-free configuration. The second common approach, refereed to as 2 % shortening, is to compute the lengths of the links in the rest location and shorten them by 2 %. This ensures that the model is prestrained in the studied configuration, however, due to the complex nature of the joint, in the rest configuration the loads no longer equate and the new rest location has to be computed numerically making the model unpredictable.

It is unclear, which approach offers more realistic approach, as, to the best of my knowledge, they never were directly compared. This would require a large reference dataset of prestrained ankle models.

2.3. Generating a reference set for testing prestrain

Including prestrain in the above model can be as simple as setting the slack lengths to different values than their lengths in the rest configuration, as shown in [5]. However, this creates an imbalanced load system in the rest configuration, and in turn changes the model in an unpredictable way. The new model may not behave as intended, however, due to its strong resemblance to the original, as seen in [5], it might serve as a reference for comparing prestrain approaches. Both its output characteristics (angular stiffness) and input parameters (slack lengths) can be obtained and are similar to those of the original model. Therefore, it can be seen as an approximation of the ankle joint itself. Furthermore, the model and its output characteristics are free from problems resulting from uncertainty in measurement and parameter acquisition.

The new model can also be prestrained the second time, by modifying slack lengths, but this time according to the common approaches used in literature - strain-free location and 2% shortening, so that they can be compared. Both methods simply require the lengths of the cables in the rest configuration of the model. In this case, the output characteristics of the model after the second prestrain can be compared to the known reference characteristics, which allows to actually ascertain, which approach is better.

Nevertheless, using only one model for this purpose is questionable, as the results might not represent a global trend. This is why, this study employs a generative approach. Namely, nearly 600 models were generated by perturbing the base model by up to ±0.5 % and ±1.5 mm in material and geometric parameters respectively. The perturbation included the slack lengths (see the rule below), effectively creating a large collection of prestrained ankle models with known reference characteristics. The perturbation values were carefully selected so that the obtained prestrained models closely resembled the base ankle model in terms of geometry, material parameters and output. These models can be considered near equivalents to actual ankle joint models and form the reference dataset for the actual comparison of prestrain approaches.

As mentioned prestraining by changing the slack lengths can be difficult as it causes unpredictable behavior of the model – it is impossible to directly control and set prestrain values. Therefore, in this study, the initial slack-length perturbation for generating the model was performed according to the following heuristic rule:

$$l_{slack,i} = l_{rest,i}\,(100 + m / 2 - Rand \cdot m) / 100 \qquad (2)$$

where: $l_{slack,i}$/ $l_{rest,i}$ – the slack/rest length of the ligament i, m – a heuristic parameter, here equal to: 5 or 7, $Rand$ – a random number from 0 to 1.

The rule was devised manually, through experimentation. For m of 5 or 7, the generated models feature low, physical levels of prestrain.

2.4. Comparing the prestrain approaches

As aforementioned, the main aim of the study was to evaluate the effectiveness of the two, common approaches to computing slack lengths: the strain-free approach and the 2 % shortening approach. To assess the quality of the two techniques, both methods were applied to every model within the generated reference dataset, described in the previous section. The obtained output characteristics from the approaches were then compared to the reference ones using a sum of absolute values of differences between the points on the angular displacement curves. The obtained values were then divided by the number of load points in the simulation. The resulting indicator represented the average angle difference between the real and prestrain curves per load point, measured in degrees.

Additionally, to further analyze the effect of prestrain, three random perturbations on lengths are also tested along with the strain-free and the 2 % shortening.

3. Results and discussion

The results section was subdivided into two parts. The first one details the generated, prestrained models of the ankle, while the second one focuses on the comparison of approaches.

3.1. The generated models of the ankle

In total, six reruns of the model generation routine were performed under different initial parameters. A model was only added to the reference dataset if it solved for the original slack length perturbation, the two typical approaches (strain-free and 2 %) and three further random perturbations.

Table 1. The details regarding the reruns for the model generation procedure, where geo_mod and mat_mod stand for the range of change for the geometric and material parameters respectively, while *m* is the heuristic parameter used in Eq (2).

id	***geo_mod* [mm]**	***mat_mod* [%]**	***m***
1	0.5	0.5	5
2	0.5	0.5	7
3	1.5	0.5	5
4	1.5	0.5	7

The reruns were summarized in Table 1. The first two trials were performed in the close vicinity of the model, with geometrical and material parameters differing only up to ±0.5mm and ±0.5 %. These values were deliberately low, as these models were supposed to be very similar to the original one, but with actual prestrain and proper reference characteristics to compare prestrain approaches.

Table 2. The average/maximal prestrain values for each ligament in the new rest location over all of the reruns, where *id* stands for the id of the run specified in Table 1.

id	***ATF* [%]**	***ATT* [%]**	***TC* [%]**	***CF* [%]**	***PTT* [%]**	***PTF* [%]**
1	1.5/5.3	0.8/4.1	1.2/3.1	1.3/2.8	1.0/5.8	1.6/6.7
2	2.1/6.2	1.1/5.9	1.7/4.0	1.8/3.9	1.4/8.1	2.2/9.8
3	1.6/6.5	0.8/8.9	1.2/3.4	1.3/3.4	0.9/6.0	1.9/8.8
4	2.2/6.7	1.1/10.2	1.6/4.2	1.8/4.3	1.3/8.5	2.6/11.6

The heuristic parameter *m* was manually selected to be either 5 or 7. These values resulted in low and realistic levels of prestrain in the generated models, as the mean prestrain never exceed 2.2 %. In some cases the values were higher, as reflected by the maximum. The actual values of prestrain are very difficult to control or predict based on the modification of slack lengths. In this study these outliers were not removed from the model dataset, due to the large overall number of generated models and realistic mean values of prestrain. Nevertheless, the outliers could also be filtered out after model generation.

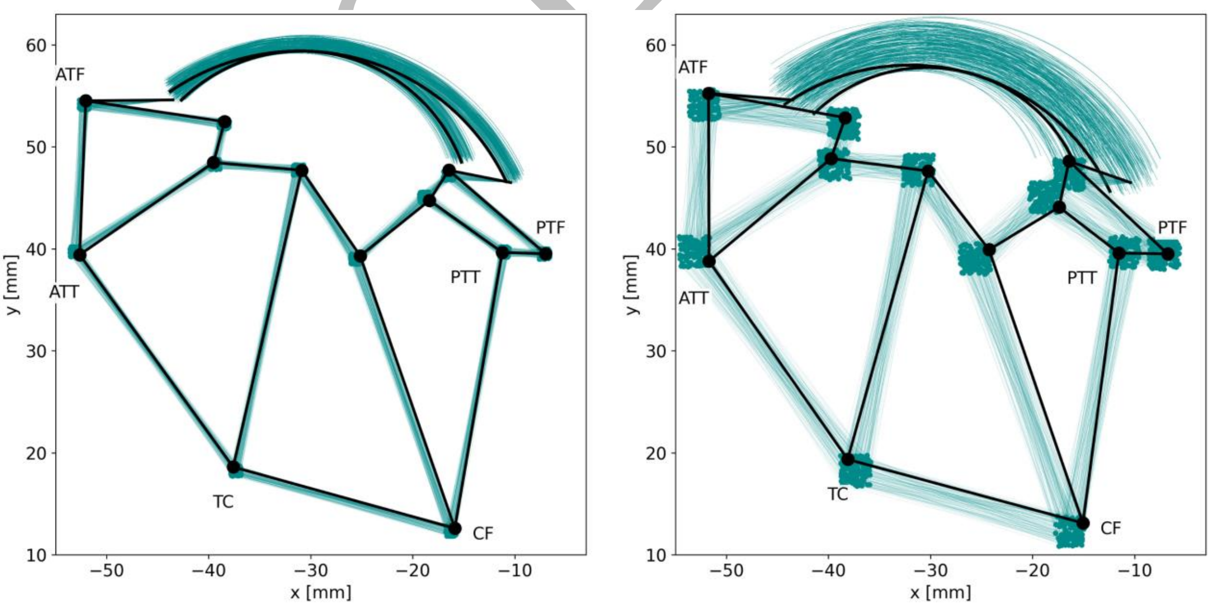

Fig. 2. The generated models that solved for all the assumed prestrain cases with bounds on the geometric parameters set to: ±0.5 mm (on the left) and ±1.5 mm (on the right). One of the models is drawn with a solid black line in both cases to showcase one of the obtained structures.

In the second batch of reruns – 3-6 – the bounds on the geometric parameters was raised to ±1.5 mm to better reflect the uncertainties in parameter acquisition, when creating models from medical scans. While the models differed significantly in this case, as seen in Fig. 2, the values of prestrain remained realistic, never exceeding 2.6 % in the mean values.

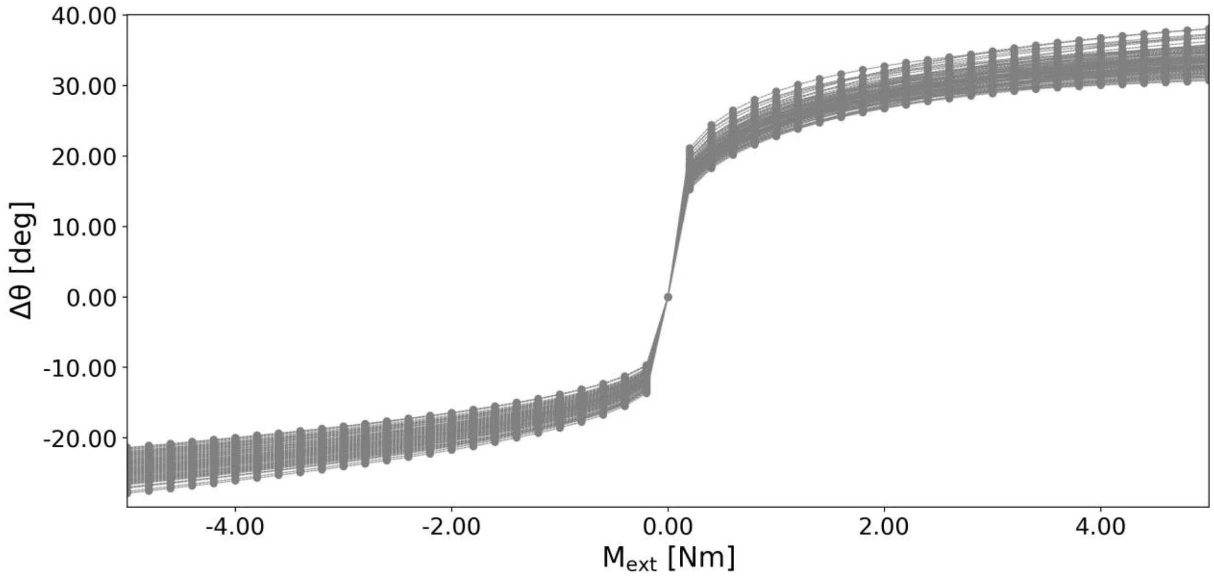

Fig. 3. The angular responses of the generated models with ±0.5 mm bounds on the geometric parameters.

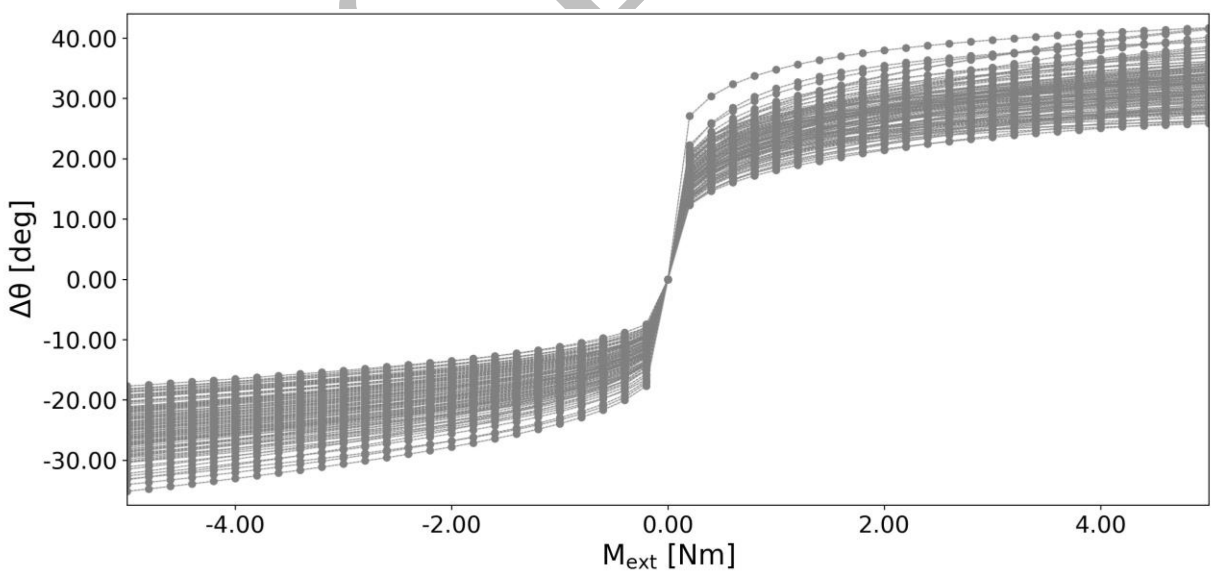

Fig. 4. The angular responses of the generated models with ±1.5 mm bounds on the geometric parameters.

In terms of their angular responses, the ±0.5 mm bounds resulted in curves close to that of the original model, as seen in Fig. 3. On the hand, the ±1.5 mm bounds returned a much higher spread of the results, although, still similar to that of the actual ankle joint, with a ratio between plantar- and dorsiflexion mostly preserved. These curves formed the reference dataset to test the prestrain approaches on.

Overall, judging by the values of prestrain and the angular responses, the procedure for generating the models was successful in creating a proper reference dataset for the actual prestrain comparison.

Nevertheless, it is worth mentioning, that solving each model for all the slack-length variants was not easy. In some cases the models did not coverage and had to be removed from the dataset. This resulted in success ratio for generating models of nearly 30 %. In total out of 2000 tested models, 592 solved for all the prestrain cases and were added to their respective reference datasets. Interestingly, with higher number of slack length perturbation, more models successfully finished the simulations.

3.2. Comparison of the prestrain approaches

As mentioned before, the model generation was only the first part of the study. These generated models, provided a much needed reference for testing the typical approaches to prestrain. Every solved model from the dataset can be prestrained with either the strain-free or 2% shortening approach and then solved again. The angular stiffness resulting from the prestrain approaches can be compared to the actual model's response, see Figs 3 and 4, simply by subtracting one curve from another and summing the results after absolute value. The smaller resulting number from the two approaches reflects an approach that is closer to reality in this case. To provide more context for comparisons, three additional approaches, in which the slack lengths were randomly shortened, were tested.

As seen in Table 3, none of the approaches returned results perfectly matching that of the reference. In fact, in all of the cases, the difference between the ground truth and the prestrain approached never dropped below 1 deg per load point. The common, 2 % shortening approach had the worst performance of all the tested cases, while random perturbations of lengths were roughly comparable to that of the strain-free approach.

Table 3. The summary of the averaged and maximal differences between the model with a prestrain approach applied with regards to its true reference response. The results are in degrees and reflect the averaged/maximal differences per load step in the model.

id		***strain-free*** **[deg]**	***2% short.*** **[deg]**	***rand. #0*** **[deg]**	***rand. #1*** **[deg]**	***rand. #2*** **[deg]**
1	*avg:*	1.32	2.05	1.11	1.40	1.12
	max:	1.55	2.97	1.87	1.64	1.86
2	*avg:*	1.79	2.07	1.58	1.79	1.59
	max:	2.38	3.66	2.71	2.48	2.71
3	*avg:*	1.32	2.51	1.37	1.38	1.33
	max:	2.72	5.16	3.88	3.98	4.31
4	*avg:*	1.73	2.30	1.62	1.70	1.57
	max:	2.06	3.13	2.09	2.24	2.13

3.3. Discussing the obtained results

The discussion of the obtained results is difficult as not many studies performed comparable numerical or practical experiments. Furthermore, the obtained results were directly linked to the underlying ankle joint model used in this study. Nevertheless, some general points could be drawn from the simulations. Firstly, the significant effect of prestrain on the angular response of the model was shown in Table 3, which was in line with a previous study on prestrain [5]. In [5], the results from the prestrain approaches were not compared to any reference curves, which limited their applicability. In the current study, the reference set of prestrained ankle model variants was generated. Due to the numerical nature of the method, the models in the dataset were properly prestrained, with no interference from uncertainty in parameter acquisition or output measurement. This allowed for a direct comparison of prestrain approaches, and revealed that for the assumed model, the strain-free approach, which essentially omits prestrain from the model, offers good overall results, in terms of the angular stiffness, strongly outperforming the more common 2 % shortening approach. Interestingly, the strain-free approach is also the simplest one to solve and analyze, as it does not change the rest configuration of the model, as shown in [5]. On the other hand, the 2% shortening approach, frequently used in ankle joint models [3], [8], [10], [22], [23], was the worst approach in all of the performed simulations. In fact, in most cases it was bested by randomly perturbing the slack lengths. Again, these results are directly applicable only to the assumed ankle model and might change when a different model is analyzed or with different bounds on the model parameters. Nevertheless, the proposed method is general and could be applied to any biomechanical model featuring ligaments. Furthermore, the results showcase how important prestrain is in a biomechanical model and how significantly it can impact the results. Finally, as every model is based on many simplifications and is only a reflection of reality, including more complex in it phenomena in it might not improve the final results.

4. Conclusions

In this study a numerical, data-driven method for comparing approaches to ligament prestrain in biomechanical models was proposed. The method was tested on a multibody model of the ankle and consisted of two steps: reference dataset generation by random sampling and prestrain comparison performed on the generated models.

The obtained results showcased that the prestrain approaches significantly affect the angular stiffness curves obtained from the model. Furthermore, the typical approach to prestrain in ankle joint modeling – 2% shortening – was proven less effective on the studied model than the simpler strain-free approach. In fact, the arbitrary shortening was worse than random perturbation of the slack lengths. Although these results should be interpreted with caution, they show that, in some cases, including more complex physical phenomena in the model might degrade the results rather than improve them, as seen in this study.

The proposed method is general and easy to apply for any biomechanical model with ligaments. It might serve as tool to explore the solution space of the model and help decide its structure.

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