SUPPLEMENTARY METHODS

A. Model Composition.

A.1. Component Overview.

We constructed a simplified model of the human triceps surae using a single, lumped, uniarticular ankle plantarflexor (PF) muscle-tendon unit (MTU). Within the MTU there was a Hill-type contractile element (CE), representing the muscle fascicles, and a series elastic element (SEE), representing tendonous tisses (i.e. Achilles' tendon and aponeuroses) [2] (Figure 2A). The extended model also included a spring in parallel with the biological MTU (Figure 2A) in order to capture the dynamics of an elastic ankle exoskeleton (EXO) (Figure 1). Details are provided here describing mathematical relations used to model components of the MTU.

A.2. Muscle (CE) Dynamics.

CE force generation was modeled in accordance with Hill-type contraction dynamics [2]. In this framework, the CE force F_{CE}, is related to the maximum CE force capacity $F_{CE_{MAX}}$, CE activation α, CE length, L_{CE}, and CE velocity, V_{CE} (Equation S1). Activation, α is normalized so that a value of unity guarantees maximum force, $F_{CE_{MAX}}$ during an isometric contraction. The length at which this maximum is achieved, L_{CE_0}, is used to normalize the CE length ($\widetilde{L_{CE}}$). $V_{CE_{MAX}}$, the shortening velocity at which the CE can no longer produce force, is used to normalize V_{CE}, which is represented as $\widetilde{V_{CE}}$.

$$F_{CE} = F_{CE_{MAX}} * (\alpha(t) * f_{\widetilde{L_{CE}}(t)^{Active}} * f_{\widetilde{V_{CE}}(t)}) + F_{CE_{MAX}} * (f_{\widetilde{L_{CE}}(t)^{Passive}}) \quad \text{(S1)}$$

The functions $f_{\widetilde{L_{CE}}(t)^{Active}}$, $f_{\widetilde{L_{CE}}(t)^{Passive}}$, and $f_{\widetilde{V_{CE}}(t)}$ characterize the normalized force-length (F-L) and force-velocity (F-V) relationships described by Zajac [2]. The active portion of the F-L curve, $f_{\widetilde{L_{CE}}(t)^{Active}}$, is defined in Equation S2. Regions of the F-L curve are defined as the steep ascending limb ($\widetilde{L_{CE}}$. < 0.75), shallow ascending limb (0.75< $\widetilde{L_{CE}}$ <.95), plateau region (0.95 < $\widetilde{L_{CE}}$<1.05), and descending limb (1.05 <$\widetilde{L_{CE}}$) per convention established by Arnold and Delp [4]. The passive portion of the F-L curve $f_{\widetilde{L_{CE}}(t)^{Passive}}$ is defined in Equation S3. Unlike the active portion of the F-L curve, which is scaled by the activation of the muscle and contributes significantly throughout the range of $\widetilde{L_{CE}}$, the passive contribution only begins to influence F_{CE} generation when $\widetilde{L_{CE}}$ > 1.0. Constants in Equation S2 and Equation S3 for the human soleus were taken from Rubenson et al. [5]

$$f_{\widetilde{L_{CE}}(t)^{Active}} = e^{-\left|\frac{\widetilde{L_{CE}}^{b}-1}{s}\right|^{a}} \quad \text{(S2)}$$

with a=3.19, b=0.87, s=0.39 and

$$f_{\widetilde{L_{CE}}(t)^{Passive}} = a * e^{b(\widetilde{L_{CE}}-1)} \quad \text{(S3)}$$

with a=2.38e-2 and b=5.31

The F-V relationship, $f_{\widetilde{V_{CE}}(t)}$ is defined by Equations S4, S5 and S6 [6, 7]. For our study, L_{CE} shortening is defined as a positive V_{CE}, while L_{CE} lengthening is defined as a negative V_{CE}.

$$V_{CE} = -\frac{\Delta L_{CE}}{\Delta t} \quad \text{(S4)}$$

$$f_{\widetilde{V_{CE+}}(t)} = \frac{1-\widetilde{V_{CE}}}{1+\frac{\widetilde{V_{CE}}}{G*V_{CE_{MAX}}}} \quad \text{(S5)}$$

$$f_{\widetilde{V_{CE-}}(t)} = 1.8 - 0.8 * \frac{1+\widetilde{V_{CE}}}{1-7.56\frac{\widetilde{V_{CE}}}{G*V_{CE_{MAX}}}} \quad \text{(S6)}$$

with G=0.17 [6].

A.3. Elastic Tissue (SEE) Dynamics.

SEE force generation was modeled with a non-linear F-L relationship. This nonlinearity exists at low forces and is referred to as a "toe region" [2, 8]. Though series elastic tissue strain patterns suggest a linear force length relationship at moderate to high forces, a non-linear model more accurately represents the requisite elastic tissue excursion to achieve such forces. Instantaneous stiffness K_{SEE} was modeled as a function of $F_{CE_{MAX}}$ and a linear tendon stiffness K_{SEE}, as seen in Equation S7 [8]. To determine the force length pattern for a given $F_{CE_{MAX}}$ and K_{SEE}, the instantaneous stiffness K_{SEE} was integrated across the range of forces to determine dL_{SEE} (Equation S8). The inverse of this result was then used to map F_{SEE} to a given L_{SEE}. The SEE could only store and return energy for L_{SEE} values above L_{SEE_0}.

$$K_{SEE} = K_{SEE}\left(1+\left(\frac{.9}{-e^{\left(\frac{Q*F_{CE}}{F_{CE_{MAX}}}\right)}}\right)\right) \quad \text{(S7)}$$

with Q=20 [8]

$$dL_{SEE}(F_{CE}) = \int_{F_{CE}=0}^{F_{CE}=F_{CE_{MAX}}} \frac{dF_{CE}}{K_{SEE}(F_{CE})} \quad \text{(S8)}$$

B. Setting Model Parameter Values.

We set parameters in the model informed by a combination of values found in the literature (e.g., [3, 9]) and values found by computer optimization (e.g., [11]) to match model output and experimental data for normal walking at 1.25 m/s (Table S1, un-bold and bold respectively).

TABLE SI: BASELINE MODEL PARAMETERS AND $\vec{M}_{bio}$ **SOLUTION**

Parameter	Value (units) (Norm.)	Source/Details
Body Mass	70 kg	Average mass of subjects from experimental data set for walking at 1.25 m/s [1]. Within 1 SD of average subject mass from Ward et al. (82.7 ± 15.2 kg) [3].
Body Height	1.70 m	Average height of subjects from experimental data set for walking at 1.25 m/s [1]. Within 1 SD of average subject height from Ward et al. (168.4 ± 9.3 m) [3].
Shank Length, L_{SHANK}	0.400 m	Set 0.03 m greater than tibial length from Ward et al. (37.1 ± 2.2 cm) [3] to include distance to femoral condyles.
$F_{CE_{MAX}}$	6000 N	Similar to approximations for soleus + med. and lat. gastrocnemius muscles used by Arnold et al. (5500.3 N) [9] and others [10-12].
$V_{CE_{MAX}}$	0.326 m/s (8.24 x L_{CE_0})	Based on values for soleus and combined gastrocnemius reported by Geyer et al. [12] and scaled using physiological cross section (PCSA) data from Ward et al. [3]
${L_{CE}}_0 / {L_{PF_{mtu}}}_0$	0.108 (unitless)	Based on fascicle lengths for soleus, med. gastrocnemius and lat. gastrocnemius reported in Ward et al. [3] and tendon slack lengths reported in Arnold et al. [9] and scaled using physiological cross section (PCSA) data from Ward et al. [3]
$\boldsymbol{L_{PF_{mtu_0}}}$	**0.366 m (0.92 x L_{SHANK})**	
$\boldsymbol{L_{CE_0}}$	**0.040 m (0.10 x L_{SHANK})**	These values (**in bold**) were all obtained using an optimization to find the morphology that would minimize error between the modeled and measured plantarflexor moment based on inverse dynamics analysis of human walking data collected at 1.25 m/s. See text for details
$\boldsymbol{L_{SEE_0}}$	**0.326 m (0.82 x L_{SHANK})**	
$\boldsymbol{K_{SEE}}$	**315.4 N/mm**	The stiffness of the SEE that resulted in the best match of model and experimental plantarflexor moment is consistent with values reported for the Achilles' tendon in the literature from both models (375.6 N/mm) [11] and experiments (188 N/mm-805 N/mm) [13-15].

*Parameters are all defined in more detail within the text. **Bold** indicates a parameter set using optimization to match model and experimental data ($\vec{\boldsymbol{M}}_{\boldsymbol{bio}}$); un-bold indicates a parameter based on values taken from literature.

First, we developed a novel geometric framework to house a 'lumped' model of the combined triceps surae (i.e. the major plantarflexors). Though the triceps surae include both biarticular (medial and lateral gastrocnemius; MG and LG) and uniarticular (soleus; (SOL)) muscles, a uniarticular configuration was chosen for the lumped model. We based the attachment geometry on a human subject with a height of 170 cm and a weight of 70 kg, to match the size and stature of the average subject from our experimental data set for walking at 1.25 m/s [1]. The length of the lower limb segment, known as the shank (Figure 2A, left) was defined by the vector intersecting the lateral and medial femoral condyles to the vector intersecting lateral and medial maleoli of the ankles, and was approximated to be 3 cm greater than the reported length of the tibia in Ward et al. (37.0±2.2 cm) to comfortably accommodate the femoral condyle [3] (Table S1). The lumped model MTU originated at 12.5% of the shank length from its proximal end and inserted distally into the calcaneal tuberosity.

We set the CE to have muscle force generating capacity of the combined triceps surae group ($F_{CE_{MAX}}$ = 6000 N) [9-11]. The maximum CE velocity, $V_{CE_{MAX}}$, was set to 8.24 x L_{CE_0} (=0.326 m/s) [12] (Table S1).

Next, we consulted a recent muscle architecture study to determine muscle-tendon (MTU) architecture values for the lumped plantarflexor model [3]. Ward et al. implemented careful dissection and MRI techniques on 21 cadavers (N=21; 9 males, 12 female; Age=83±9 years; height=168.4±9.3 cm; weight=82.7±15.3 kg) to comprehensively quantify average skeletal lengths, muscle body length, muscle fascicle length, pennation angles, and physiological cross-sectional areas (PCSA) of lower limb muscle bodies. Elastic features beyond the muscle bodies, such as external tendons and tendinous attachments, were not reported and were excised prior to muscle body measurement. Arnold and Delp used Ward's skeletal and muscle body data and extrapolated elastic tissue lengths to fit origin and insertions of the respective muscles [9]. Thus, we took average muscle fascicle rest lengths from Ward et al. and divided by the total muscle-tendon slack length estimates presented in Arnold and Delp for the muscles in the triceps surae group, and used their respective PCSAs to determine a weighted averaged fraction of muscle to muscle-tendon unit length for the tricep surae ($L_{CE_0}/{L_{PF_{mtu}}}_0$). A weighted average according to PCSA was also used to determine the pennation angle of our lumped plantarflexor model. The resultant $L_{CE_0}/{L_{PF_{mtu}}}_0$ was then multiplied by the cosine of the pennation angle to yield a lumped $L_{CE_0}/{L_{PF_{mtu}}}_0$ fraction of 0.108. With this subset of parameters constrained based on literature values (Table S1, unbold), we moved on to use computer optimization to set the remaining parameter values based on matching model outputs to experimental data from normal walking at 1.25 m/s (Table S1, bold).

C. *Finding the $\vec{M}_{bio}$ Solution.*

First, we defined a muscle-tendon unit (MTU) morphology vector $\vec{M}$, containing the set of remaining model parameters: [${L_{PF_{mtu}}}_0$, L_{CE_0}, L_{SEE_0}, K_{SEE}]. Then we set up a constrained optimization problem with the goal to find the morphology vector, $\vec{M}$ that would minimize the difference between the plantarflexor moment generated by our lumped model, $m_{model_{PF}}$, and the experimental net ankle moment, m_{net} measured during walking at 1.25 m/s. We called this optimal morphology vector, $\vec{M}_{bio}$., as it should be most representative of the underlying physiology of the biological system.

We applied three physiologically relevant constraints to make the optimization problem more tractable. First, based on literature values for typical plantarflexor MTU morphology we enforced $L_{CE_0}/L_{PF_{mtu_0}}$= 0.108 (see Supp. Section B, Table S1). Next, we constrained the model to follow the ankle joint kinematics and kinetics [1] as well as the muscle fascicle (CE) strain pattern [5] reported in previously published studies of normal walking at 1.25 m/s. Briefly, stride average ankle angle and net moment data were computed by combining motion analysis techniques, force ergometry and inverse dynamics calculations and averaged across 9 healthy subjects (N=9; 5 males, 4 females; mass=80.3 ±14.7 kg; height=170 ±3 cm; leg length=92±2 cm) who walked on a motorized treadmill at 1.25 m/s [1]. The CE strain data were collected using ultrasound imaging techniques from the right soleus muscle of 8 healthy subjects (N=8; mass=70.3 ±9.2 kg) walking on a motorized treadmill at 1.20 m/s (not shown) [5].

These constraints made it possible to follow a sequence of calculations for a given morphology vector, $\vec{M}$ ($L_{PF_{mtu_0}}$, L_{CE_0}, $L_{SEE_0}$and K_{SEE}) and evaluate its performance. First we used the ankle angle constraint and the model's defined joint geometry (Figure 2a, Table S1) to determine $L_{PF_{mtu}}(t)$, the distance between the insertion and origin of the lumped MTU at each instant over a walking stride. Since the MTU consists of the CE and SEE in a series configuration,

$$L_{PF_{mtu}}(t) = L_{SEE}(t) + L_{CE}(t) \tag{S9}$$

Equation S9 holds true for *all* MTU morphologies. Next, for a given $L_{PF_{mtu_0}}$, we could determine a L_{CE_0} using the $L_{CE_0}/L_{PF_{mtu_0}}$= 0.108 constraint, and per Equation S9, an L_{SEE_0} was concurrently defined. Then, we used the muscle fascicle (CE) strain pattern constraint and L_{CE_0} to determine the absolute CE length, $L_{CE}(t)$ and applied Equation S9, to determined $L_{SEE}(t)$ for all time points over the stride. Next, with a given K_{SEE}, we applied the SEE force-length dynamics described in Equations S7 and S8 to calculate tendon force F_{SEE} at each L_{SEE} and since the CE and SEE are in series, we assumed that

$$F_{CE}(t) = F_{SEE}(t) = F_{PF_{mtu}}(t) \tag{S10}$$

for all time points in the stride. The resulting $F_{PF_{mtu}}(t)$ was then applied across the moment arm defined by the model geometry (~4.1 cm on average) to determine the lumped plantar flexor moment for that given morphology vector, $m_{model_{PF}}(\vec{M})$.

Finally, the $m_{model_{PF}}(\vec{M})$ was assessed against the net ankle moment profile experimental data m_{net} at each of *n* data points across the stride by calculating a conditional root mean square error, or RMSE (Equation S11).

$$RMSE = \sqrt{\frac{\sum_{t=1}^{n}(m_{model_{PF}}(\vec{M})(t) - m_{net}(t))^2}{n}} \tag{S11}$$

Because the tricep surae muscle group can only produce moments in the plantar flexion direction, RMSE was only calculated where the m_{net} was greater than 0 N-m and inflated by 5 N-m for time points in the 35%-50% portion of the stride, where contributions from antagonist muscles (e.g., tibialis anterior) to overall net ankle moment are likely negligible.

Using the framework and constraints described above, we used the *fminsearch* function in MATLAB (Mathworks Inc.; Natick, MA) to find the optimal morphology vector, $\vec{M}_{bio}$ that minimized the RMSE (Equation S11). The optimization resulted in the solution vector $\vec{M}_{bio}$ = [$L_{PF_{mtu_0}}$, L_{CE_0}, L_{SEE_0}, K_{SEE}] = [.366 m, 0.04 m, 0.326 m 315.4 N/mm] which had a RMSE value of 10.7 N-m (Table S1, bold).

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