**\paragraph{Joint reaction forces and moments analysis.}** Since the equations of motion of the musculoskeletal model were formulated in terms of the generalized coordinates and generalized forces, the internal forces and moments were not solved while performing the computed muscles control or residual reduction algorithm simulations. Consequently, we employed a/the joint reaction analysis provided by OpenSim to compute the resultant forces and moments between two consecutive bodies in the kinematic chain connected via a joint. The contact forces and moments of joints were obtained by formulating them through the Newton-Euler equation of motion and solving them recursively from the distal to proximal joints.\\

The free body diagram of $i$th body and joint is provided in Figure \ref{Fig\_JRF\_FBD}, which has been adopted from the figure represented in the Supplementary Material of \cite{151}. The Newton-Euler formulation for $i$th body can be represented as Eqn. \eqref{Eqn\_Body\_Reaction\_Force} as adapted from \cite{151}, which was solved to obtain the contact forces and moments acting on the body.

\begin{equation}\label{Eqn\_Body\_Reaction\_Force}

\end{equation}

\begin{figure\*}[!t]

\end{figure\*}

where $M\_i(q)$ and ${\mathit{\mathbf{a}}}\_i$, respectively, represent the mass matrix of the body $i$ and vector of the linear and angular acceleration of body $i$ expressed at ground frame, and $F\_{constaint}$ accounts for the forces applied by constraints, if applicable. Through this equation $F\_{muscle}$, $F\_{external}$, and $F\_{gravity}$ represent the force and moment applied by a muscle, forces applied externally (e.g. ground reaction forces and moments), and gravitational forces applied to the body, respectively. Lastly, $R\_{i+1}$ accounts for the applied reaction forces from the $(i+1)$th to the $i$th joint.\\

Since these reaction forces and moments are expressed at the origin of the body frame to include all terms in a common reference frame, they need to be transformed to the location of the joint frame (i.e. offset frame), where the joint has been defined between two consecutive bodies as represented in Eqn. \eqref{Eqn\_JointReactionForce} \cite{151}.

\begin{equation}\label{Eqn\_JointReactionForce}

\end{equation}

The vectors of $F\_i$ and $\tau\_i$ represent the joint reaction force applied to the joint of interest expressed at the ground frame.\\

As was mentioned earlier, this analysis was adopted from the supplementary material of \cite{151}, and we reference the readers to this paper for detailed discussion about this analysis.\\

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**\*\*\*\*\* ALREADY CHECKED\*\*\*\*\***

**\subsection\*{Modeling and simulation of assisted subjects}**

The kinematics of the exoskeletons were already discussed; in order to model ideal exoskeletons in OpenSim framework, we used the Torque Actuators provided by OpenSim API\cite{103}. Torque actuators of the biarticular and monoarticular exoskeletons were assigned, as shown in Figure \ref{Fig\_Exos\_Model\_Opensim}.

\begin{figure\*}[h!]

\end{figure\*}

As is represented in Figure \ref{Fig\_Exos\_Model\_Opensim} \subref{Fig\_Bi\_Exo\_Model\_Opensim}, both torque actuators of the biarticular exoskeleton were assigned to the torso; the reaction forces of the actuators were then applied to the torso, which matches the kinematics and dynamics model of the biarticular exoskeleton.

\begin{align}\label{Eqn\_Biarticular\_Torque\_Act}

\end{align}

The onoarticular exoskeleton (Figure \ref{Fig\_Exos\_Model\_Opensim} \subref{Fig\_Mono\_Exo\_Model\_Opensim}) was modeled by assigning the hip joint actuator from the torso to the femur body and the knee joint actuator was assigned from the femur to the tibia body at which the reaction torque of the knee torque applied to femur body:

\begin{align}\label{Eqn\_Monoarticular\_Torque\_Act}

\end{align}

\paragraph\*{Computed muscle control adjusted objective function.} To investigate the performance of the assistive devices and their effect on the human musculoskeletal system through the OpenSim simulation framework, we used the CMC algorithm. The computed muscle control algorithm objective function depends on the sum of squared muscle activation and reserve actuators, which compensates for modeled passive structures and potential muscle weakness\cite{93}:

\begin{equation}\label{Eqn\_CMC\_Normal\_Obj\_Func}

\end{equation}

where $w\_i$ determines the weight of reserve actuators, which is generally selected as a small number to highly penalize the use of reserve actuators. By adding assistive device actuators (i.e. Torque Actuators) to the musculoskeletal model of the subject, they are added to the CMC tool objective function.\\

The adjusted objective function includes the assistive actuators as is expressed in Eq. \eqref{Eqn\_CMC\_Assisted\_Obj\_Func}, and by selecting proper weights for the assistive actuators, they can be chosen by the optimizer as the actuation of the assigned degree of freedom.

\begin{equation}\label{Eqn\_CMC\_Assisted\_Obj\_Func}

\end{equation}

In the adjusted objective function, $w\_{exo,i}$ is torque actuator weights, which is named optimal force in OpenSim \cite{93} penalizing the usage of torque actuators. By selecting a large number, penalization of the actuators is insignificant and they are selected for actuating the joint between two bodies assigned for the torque actuator. If we select a small optimal force, the optimizer will highly penalize the usage of exoskeleton actuators. To study each configuration of the exoskeleton at their maximum performance, the assigned torque actuator's optimal force was selected as 1000 N.m enabling the optimizer to use the assistive actuators as much as possible during a gait cycle simulation.\\

**\paragraph\*{Power calculation of metabolics and actuators.}** Similar to the unassisted procedure, the instantaneous metabolic power of the subjects was computed using the energetic model of Uchida et al. \cite{106}. The metabolic rate of each subject was then derived through integration of the metabolic power over the gait cycle. In order to compute the energy consumption of the assistive actuators, the power profile of the actuators was obtained and their absolute power profiles were integrated over the gait cycle and normalized to the mass of the subject. Similar to the power consumption of the exoskeleton procedure, the negative power or regeneratable power through a gait cycle was calculated by obtaining the negative power profile and integrating it over the gait cycle and normalizing it to the mass of the subject.\\

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

**\paragraph{Joint reaction forces and moments analysis.}** We performed a similar joint reaction force analysis to study the effect of the assistive devices on the reaction forces and moments of assisted and unassisted joints. Nonetheless, appending assistive devices to the musculoskeletal system modifies the Newton-Euler equations of motion of bodies to which the Torque Actuators were appended ( i.e., Eqn.\eqref{Eqn\_Body\_Reaction\_Force}), as expressed in Eqn. \eqref{Eqn\_Body\_Reaction\_Force\_Modified}.

\begin{equation}\label{Eqn\_Body\_Reaction\_Force\_Modified}

\end{equation}

where $\sum{\mathit{\mathbf{F}}}\_{\mathrm{assistive}}$ represents the applied or reaction torques of the assistive actuators.

**\subsection\*{Simulations of Multi-criteria Optimization}**

The optimization stage of the computed muscle control (CMC) algorithm uses the weighted sum of squares to solve the reduncancy of muscles and assigned actuators to select a set of actuations with the most economical cost for tracking the kinematics of the dynamic model of the subject \cite{92}. To investigate the maximum effect of assistive devices on the metabolic power consumption of assisted subjects, regardless of the power expenditure of devices, large weights were assigned to the assistive actuators.\\

However, in real-time applications, the exoskeletons are restricted by the power that can be supplied to their actuation modules and the maximum assistive torque that the actuation modules can provide to the joints of interest. To study the performance of the purposed devices under constrained maximum torques that the assistive actuators can provide to the joints and their effect on the musculoskeletal system with lower power demands, we adopted a Pareto method for a multi-criteria concept\cite{113} and implemented it through the/our musculoskeletal simulation framework.\\

The adopted Pareto method integrates all optimization criteria in its procedure and constructs a Pareto front representing non-dominant solutions among the criteria, enabling us to obtain optima curves for each configuration of the devices \cite{107} and conduct a fair comparison between the exoskeletons and load conditions. In this study, the metabolic cost reduction and power consumption of the assistive actuatorswere considered as two optimization criteria to study and compare different configurations of the exoskeletons in both load conditions.\\

One of the acceptable Pareto fronts is a discrete set of Pareto-optima points, obtained by constructing a single objective function by integrating objectives and optimizing the single cost function throughout the specific range of values of the parameters used to combine the cost functions into a single objective function \cite{108}.\\

The Pareto optimization method has been used by M. L. Handford and M. Srinivasan\cite{111,127} to study robotic lower limb prostheses by simultaneously optimizing the metabolic and prosthesis cost rates. \\

**\paragraph\*{The workflow of the simulations.}** To perform the simulations of the Pareto-optimization in the OpenSim framework, we constrained the peak torque of assistive actuators throughout a specific range of torque they can provide during a gait cycle, which constrains the objective function mentioned in Eq \eqref{Eqn\_CMC\_Assisted\_Obj\_Func} and changes the solution of the optimizer for the muscles and actuators redundancy problem. This variation over a discrete range of the maximum torque that assistive actuators can provide results in several solutions on the optimization objectives space. By filtering these Pareto curves and obtaining the non-dominant solutions, we achieved a/the Pareto front for each configuration of the exoskeleton under both load conditions.\\

For both the biarticular and monoarticular exoskeletons, the maximum torque that their actuators could provide to the hip and knee joints was varied between 30 N.m and 70 N.m. The simulations of this phase were performed by fixing the maximum torque that the hip actuator can provide and varying the constraint of the knee over the specified range. After conducting simulations of exoskeletons with a fixed hip constraint and varying knee constraint, the maximum torque limit of the hip actuator was modified to perform the next iteration of the simulations. The algorithm is shown in the following pseudo-code.\\

\begin{algorithm}\label{Algorithm\_Pareto\_simulation}

\end{algorithm}

**\paragraph\*{Regeneration effect on the efficiency of optimal devices.}**

The regeneratable power of the optimal exoskeletons can be acquired by capturing the negative power profiles of assistive actuators and obtaining the dissipated energy from the negative power profile. This dissipated energy was normalized by the mass and gait duration of each subject and trial. Although the maximum reported efficiency of harvesting dissipated power has ranged between 30\% to 37\% for the lower limb assistive devices \cite{140}, the MIT cheetah custom design \cite{144,145} and the biomechanical energy harvester developed by Donelan et al. \cite{143} reported and experimentally verified 63\% regeneration efficiency. Hence, we examined the performance of our devices from the perspectives of various efficiency factors and selected 65\% as energy harvesting efficiency for the analyzed exoskeletons, which is the maximum efficiency that has been reported for regeneration. The regeneration effect on the simulated configurations of devices and their optimal trade-off were studied by subtracting the regeneratable power from the total power consumption of the/our devices.\\

**\paragraph\*{Root mean square error of profile in gait phases.}** To establish quantitative and systematic comparisons between two profiles of selected optimal devices, we obtained the root mean square error (RMSE) between overall and phases of profiles. The phases of a general gait cycle were adopted from \cite{150,161} and customized for each subject and trial according to their toe-off timing, as represented in Figure X in \nameref{S2\_Fig}. The gait cycle of each subject and trial was then partitioned to its phases, and we used the root mean square error (RMSE) method to compute the difference between the two profiles in each phase of the gait cycle and reported them by their mean and standard deviation over the subjects.

**\subsection\*{The Effect of Optimal Device Inertial Properties on Subject Energetics}**

The mass and inertia of the proposed biarticular and monoarticular exoskeletons affect the waist, thigh, and shank segments. As discussed in the Kinematic Modeling section, the biarticular exoskeleton is designed to deliver the assistance distally to the knee joint. This property of the biarticular exoskeleton enables designers to attach the knee actuation module to the waist instead of the thigh, which is the main difference between the inertial properties of the two proposed exoskeletons. Nevertheless, it should be noted that the reflected inertia of the knee actuation module in both exoskeletons is applied on the shank regardless of its grounded segment.\\

To computationally study the effect of the inertial properties of the exoskeletons on the metabolic rate of assisted subjects, we assigned two identical masses and centers of mass measured from the hip joint for the links attached to the thigh and shank. Moreover, a typical and identical inertia and mass were selected for the actuation module of both exoskeletons. Additionally, the maximum achievable torque of the actuator was set to 2 N.m, which can be provided by MaxonMotor EC90 Flat 260W, and the required transmission ratio was calculated by dividing the peak torque at the joint level into the peak torque of the actuator. The reflected inertia was then computed using Eqn.\eqref{Eqn\_reflected\_inertia}.\\

\begin{equation}\label{Eqn\_reflected\_inertia}

\end{equation}

The inertia of the moving segments (i.e., thigh and shank segments) was computed by considering the distal mass effect on the inertia, reflected inertia of the actuation module, and the leg inertia provided by \cite{133}, which was calculated about the hip joint in the body frame. Eqn.\eqref{Eqn\_segment\_inertia} represents the inertia calculation of the moving segment.

\begin{equation}\label{Eqn\_segment\_inertia}

\end{equation}

The mass, the center of mass, and inertia used for the numerical simulations are represented in Table \ref{Table\_Exokeletons\_Mass\_Inerta}. The mass of each segment is within the range of the weight of the exoskeletons studied by Mooney et al.\cite{41} for calculating the augmentation factor. The center of mass for each segment was mostly chosen based on the mean length of the thigh and shank segments\cite{136} under the assumption of unity distribution of link weight.\\

\begin{table}[ht]

\end{table}

The metabolic model proposed by Browning et al. \cite{133} calculates the metabolic rate of the subject with a loaded segment; however, since we were interested in the effect of inertial properties of the exoskeletons on the change of the metabolic rate, we adopted and modified the model by subtracting the metabolic rate of the unassisted subject from the subjects wearing the devices. The equations of the final model used to analyze the effect of the inertial properties of the exoskeletons on the metabolic rate are provided in Eqn.\eqref{Eqn\_AddingMass\_MetabolicRate} and \eqref{Eqn\_AddingInertia\_MetabolicRate}, respectively.

\begin{equation}\label{Eqn\_AddingMass\_MetabolicRate}

\end{equation}

\begin{equation}\label{Eqn\_AddingInertia\_MetabolicRate}

\end{equation}

The effect of the mass and inertia of the exoskeletons on the metabolic cost of the subjects was reflected on the Pareto curves and filtered to obtain the Pareto front curves with the effect of the exoskeleton inertial properties on the metabolic expenditure.\\

**\paragraph\*{Modified Augmentation Factor.}** In studying selected cases from the solutions of the Pareto front curves, a more systematic analysis of the performance of devices under the effect of their inertial properties that can be employed for both {\it loaded} and {\it noload} conditions is desirable. Consequently, we used an/the augmentation factor \cite{41} with some primary modifications.\\

The augmentation factor (AF) was developed by Mooney et al. \cite{41} to address the limitations of the performance index introduced by Sawicki and Ferris \cite{149} to measure the relationship between the device applied positive power and change in metabolic power consumption. The augmentation factor was established to estimate metabolic power change due to carrying the exoskeleton, which balances the mean positive power, resulting in a metabolic improvement and net dissipated power and device weights, causing metabolic detriment.\\

Although the augmentation factor resolved difficulties in the previous performance metrics and introduced a general factor for predicting the performance of assistive devices, it did not address the effect of inertia caused by the actuation unit and attached masses in moving segments. The study accomplished by Browning et al. \cite{133} noted the importance of the inertia effect on the metabolic burden of subjects, showing the necessity of including this factor for any performance measurement of exoskeletons.\\

The modified augmentation factor (MAF) was introduced to address this central issue of the augmentation factor. In order to include the inertia effect in the augmentation factor, we adopted the model developed by Browning et al. \cite {133} to estimate the metabolic power ratio change due to the inertia ratio change of subjects walking while wearing weights on their lower limbs to subjects walking without any load. We then performedsimple algebraic manipulations to obtain the device location factor ($\gamma\_{i}$) for the inertia applied to each segment, as is represented in Eqn.\eqref{Eqn\_Inertia\_Factor}. It is noteworthy to mention that $\gamma\_{i}$ was obtained under the assumption of device inertia in addition to the inertia of a/the unloaded leg.

\begin{equation}\label{Eqn\_Inertia\_Factor}

\end{equation}

In this inertia position factor represented in Eqn.\eqref{Eqn\_Inertia\_Factor}, $A\_i$ is the multiplier of $I\_{ratio}$ in Browning models for foot, thigh and shank segments and $I\_{unloaded}$, $m\_{subjects}$, and $MC\_{unloaded}$ are the inertia of leg without any external load, mean weight of subjects, and metabolic rate of subjects walking without any load on their segments respectively which were obtained from the \cite{133} models and plots. The modified augmentation factor (MAF) was obtained by adding the effect of inertia on the metabolic detriment part of this factor, and it can be expressed as Eqn.\eqref{Eqn\_MAF}.

\begin{align}

\end{align}

Where $p^{+}$, $p^{-}$, and $p^{disp}$ are representing mean positive, negative, and dissipated power calculated through Eqn.\eqref{Eqn\_disp\_power}. The $\beta\_i$ in MAF stands for the location factor of the device mass which is 14.8, 5.6, 5.6, and 3.3 $W/kg$ from the foot to waist respectively \cite{41,133} and $\gamma\_j$ is representing the location factor of the device inertia which is 47.22, 27.78, and 125.07 $W/{kg.m^2}$ from the foot to thigh respectively. Consistent with augmentation factor procedure \cite{41}, MAF uses muscle-tendon efficiency,$\eta = 0.41$ to convert the mechanical assistive power to metabolic power determined empirically by Sawicki and Ferris\cite{149} and Malcolm et al.\cite{40}. Finally, we normalized modified augmentation factor by the weight of each subject.

**\subsection\*{Validation of Simulations}**

The comprehensive validation procedure of the OpenSim simulations was published by Hicks et al. \cite{92} in which they explained how to validate modeling and simulation results at each stage. Additionally, Dembia et al. \cite{93} explained simulation verification for their simulations of assistive devices, and we followed the same procedures explained in \cite{92,93} to validate our results from the simulations.\\

As is already discussed, the adjusted model, adjusted kinematics, and processed ground reaction forces provided by \cite{93} were used for accomplishing this study, which was evaluated and validated by Dembia et al. \cite{93}. The muscular activation resulting from the simulations of unassisted subjects was validated with the experimentally recorded electromyography (EMG) signals \cite{92,93} in which there were some timing and magnitude discrepancy between simulated and experimentally collected activation of some muscles which was due to excessive passive forces in knee and ankle joints.\\

The \textit{loaded} and \textit{\textit{noload}} joint kinematics and kinetics were compared with the results of the studies accomplished by Huang and Kuo \cite{131} and Silder et al.\cite{132} and validated qualitatively. Since our simulations of the unassisted subject for \textit{loaded} and \textit{noload} conditions were the same with Dembia et al. simulations, we reproduced their simulations and compared them with their results to validate our reproduced simulations results. Additionally, since we used the provided RRA results for performing the CMC simulations, the joint moment and joint kinematics represented in this paper were already validated.\\

The other source of error during the simulations is kinematics error, which was analyzed to be in the recommended thresholds by Dembia et al.\cite{93}. Since the inverse kinematics stage of the simulation was not reproduced in this study, the markers error was not examined, and we relied on the previously performed verification on this error source. The analysis of Dembia et al. \cite{93} on residual errors showed that the residual forces lie below the threshold recommended by Hicks et al. \cite{92}; however, the residual moments exceeded from the Hicks et al. thresholds but since the joints moment were matching with \cite{92}, it was claimed that these exceeding residual moments do not affect the interpretations \cite{131,132}.

Another error source in these simulations could be additional moments introduced to compensate any unmodeled passive structures and muscle weakness, which were checked to be in their recommended thresholds to have less than 5\% of net joint moments in peak and RMS \cite{93}.\\

To ensure that our simulations in both ideal and Pareto-optimization phases did not deviate from the defined error source thresholds, we analyzed the kinematics of all simulations and checked their divergence from the adjusted kinematics resulted from the RRA simulations. Additionally, some simulations of the Pareto-optimization part were selected randomly, and their residual and reserve moments and forces were analyzed.

**\subsection\*{Performance Metrics}**

For the purpose of having methodical analysis and comparison between the assistive devices and load conditions, some performance metrics were defined. As discussed earlier, the ultimate goal of each assistive device is reducing energy consumed by the subject for performing a task that was walking with and without load at self-selected speed in this study.

Therefore, we calculated the normalized gross whole-body metabolic rate of the subjects in two different assistive devices and load conditions, and then metabolic cost reduction was computed using the metabolic rate of assisted and unassisted subjects. This procedure of metabolic cost calculation was repeated for all seven subjects in three trials to obtain the total average metabolic energy expenditure and metabolic cost reduction for each assistance scenario and load condition.\\

Another important metric for assessing the performance of an exoskeleton is the power it consumes to assist the subjects. To analyze this metric in the simulated exoskeletons, we computed the absolute power consumed by all actuators, and the reason for considering the absolute value is the absence of the regeneration mechanism as a general case for the exoskeletons. Additionally, to analyze the amount of power available for regeneration, we computed the negative energy of the exoskeletons. The power consumption metric is a crucial part of the exoskeletons analysis to estimate their efficiency and battery life for untethered devices.

At the Pareto optimization part of the study, these two introduced metrics (i.e., metabolic cost reduction and power consumption) were optimized simultaneously, and their set of optimal solutions was represented for each device and load condition. This Pareto front represents the set of different configurations for each exoskeleton in terms of power consumption and the assistance the device can provide. For more detailed analyses, some specific configurations in each exoskeleton and load condition have been selected and studied exhaustively.\\

Additionally, the regeneratable power and inertial properties of the exoskeletons, as two critical metrics for analyzing the performance of the assistive devices, have been studied in simulations of multi-criteria optimization by reflecting their effect on the Pareto-curves and obtaining the Pareto sets under the effect of these two metrics.

Some muscular activations of the lower limb key muscles were extracted and studied to gain insight into how an assistive device can change muscle activities and, consequently, metabolic cost resulting from muscle activities.

Lastly, the reaction forces and moments of the joints were computed to gain insight into the effect of assistive devices on the reaction forces of the joints and understand how the proposed device and the monoarticular exoskeleton can change the reaction forces and moments of the joints.

**\subsection\*{Statistical Analysis}**

To conduct methodical comparisons among scenarios with the discussed metrics, we employed statistical analyses. Since the simulations were performed on seven subjects with three trials in five different scenarios, repeated measures analysis of variance (ANOVA) and Tukey Post-hoc were applied to test the statistically significant difference between the selected metrics and scenarios. Additionally, for the Pareto simulations, the statistical analysis has been performed for the specific points selected from the Pareto front for further investigation. Nevertheless, the standard deviation of all points on the Pareto front was explicitly plotted for both criteria. We used a significance level of 0.05 and SPSS \cite{spss} for performing the tests.