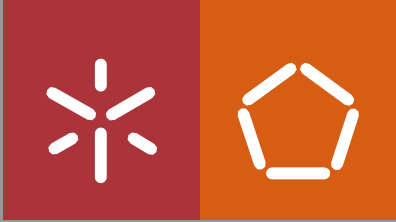




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Universidade do Minho
Escola de Engenharia

Development of an Advanced Multibody
Musculoskeletal Model of the Human Movement to
Improve Device-Assisted Gait: Application to Mobility
Solutions





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**Development of an Advanced Multibody
Musculoskeletal Model of the Human
Movement to Improve Device-Assisted Gait:
Application to Mobility Solutions**

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Trabalho realizado sob a orientação de

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"If I have seen farther than others, it is because I was standing on the shoulders of giants."

Isaac Newton

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Muito, muito obrigada!
Mariana Rodrigues da Silva

STATEMENT OF INTEGRITY

I hereby declare having conducted this academic work with integrity. I confirm that I have not used plagiarism or any form of undue use of information or falsification of results along the process leading to its elaboration.

I further declare that I have fully acknowledged the Code of Ethical Conduct of the University of Minho.

RESUMO

Desenvolvimento de um Modelo Multicorpo Musculoesquelético Avançado do Movimento Humano para a Melhoria da Marcha Assistida por Dispositivos Auxiliares: Aplicação a Soluções de Mobilidade

A biomecânica do movimento humano é uma área de investigação multidisciplinar que envolve o estudo dos aspetos mecânicos do corpo humano e o impacto que as forças têm no movimento dos segmentos anatómicos. A utilização de ferramentas computacionais para compreender o comportamento dinâmico do movimento humano tem vindo a aumentar devido à vasta gama de aplicações existentes para melhorar o desempenho humano ou tratar lesões. O conhecimento deste tópico pode fornecer opções promissoras para o desenvolvimento de dispositivos auxiliares adaptados às necessidades dos pacientes. O relatório de 2022 da Organização Mundial de Saúde (OMS) e do Fundo das Nações Unidas para a Infância (UNICEF) estima que mais de 2,5 mil milhões de pessoas em todo o mundo utilizam um ou mais dispositivos auxiliares, prevendo-se que este número aumente para 3,5 mil milhões em 2050. Para além disso, a utilização incorreta e prolongada de dispositivos auxiliares tem consequências prejudiciais para os doentes, incluindo o desenvolvimento de problemas de saúde secundários. Assim, este trabalho utiliza ferramentas computacionais para desenvolver um modelo multicorpo musculoesquelético avançado do movimento humano para investigar a marcha assistida por dispositivos.

São desenvolvidas várias metodologias no âmbito do contexto de sistemas multicorpo para atingir o objetivo pretendido. É apresentada uma nova formulação para o complexo articular do tornozelo, que utiliza uma junta universal modificada incorporada com um *massless link*. É também proposta uma metodologia para restringir a amplitude de movimento das articulações. Momentos de resistência são aplicados aos corpos para reproduzir o comportamento dissipativo dos materiais que constituem as juntas e para evitar configurações inaceitáveis dos corpos. Dados experimentais do movimento humano foram adquiridos no Laboratório de Biomecânica de Lisboa e a formulação de cinco guiamentos, desenvolvidos para guiar os graus de liberdade de sistemas biomecânicos multicorpo, é explicada em pormenor. A modelação computacional dos músculos esqueléticos humanos foi conseguida utilizando uma variante do modelo de Hill, que é composto por um elemento contrátil ativo organizado em paralelo com um elemento elástico. A dinâmica da contração muscular e os procedimentos de otimização são descritos. São desenvolvidos dois modelos tridimensionais biomecânicos multicorpo do corpo humano, que diferem na complexidade da articulação do ombro. Colaborações com o Centro de Reabilitação do Norte e a ORTHOS XXI foram estabelecidas para reforçar o trabalho computacional relacionado com a marcha assistida por dispositivos auxiliares. Foram também adquiridos dados experimentais deste tipo de marcha. De acordo com as conclusões da revisão da literatura realizada neste trabalho, são investigadas várias abordagens para analisar as interações dispositivo-modelo e dispositivo-solo. Todas as metodologias propostas neste trabalho são integradas num caso de aplicação final para validação.

Palavras-chave: Biomecânica do movimento; Dinâmica de sistemas multicorpo; Marcha humana; Dispositivos de auxílio à marcha; Canadianas.

ABSTRACT

Development of an Advanced Multibody Musculoskeletal Model of the Human Movement to Improve Device-Assisted Gait: Application to Mobility Solutions

Biomechanics of human motion is a multidisciplinary field of investigation that involves the study of the mechanical aspects of the human body and the impact that forces have on the movement of the anatomical segments. The use of computational tools to understand the dynamic behavior of the human movement has been rising due to the wide range of applications to improve the human performance or to treat injury. The knowledge on this topic may provide promising options for the development of assistive devices tailored to the needs of patients. The 2022 report of the World Health Organization (WHO) and the United Nations Children's Fund (UNICEF) estimates that more than 2.5 billion people globally use one or more assistive devices, and this number is expected to rise to 3.5 billion in 2050. In addition, the incorrect and prolonged use of assistive devices has harmful consequences for patients, including the onset of secondary health conditions. Hence, this work uses computational tools to develop an advanced multibody musculoskeletal model of the human movement to investigate device-assisted gait.

Several methodologies are developed within the framework of multibody systems to achieve the intended aim. A new formulation for the ankle joint complex is presented, which uses a modified universal joint incorporated with a massless link. A methodology to restrict the range of motion of joints is also proposed. Joint resistance moments are applied to the connected bodies to mimic the dissipative behavior of the joint materials and to prevent unacceptable configurations of the bodies. Experimental data of the human movement was acquired at the Lisbon Biomechanism Laboratory and the formulation of five different driving constraints developed to guide the degrees-of-freedom of biomechanical multibody systems is explained in detail. The computational modeling of the human skeletal muscles is achieved by using a variant of the Hill model, which is composed of an active contractile element arranged in parallel with an elastic element. The muscle contraction dynamics and optimization procedures are described. Two three-dimensional biomechanical multibody models of the human body are developed, which differ in the complexity of the shoulder joint. Collaborations with *Centro de Reabilitação do Norte* and ORTHOS XXI were established to strengthen the computational work on device-assisted gait. Experimental data of assisted gait was also acquired. According to the findings of the literature review conducted on this thesis, several approaches to deal with the device-model and device-ground interactions are investigated. All methodologies proposed in this work are integrated into a final application case for validation.

Keywords: Biomechanics of motion; Multibody dynamics; Human gait; Assistive devices; Crutches.

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LIST OF ABBREVIATIONS

2D	Two-Dimensional
3D	Three-Dimensional
Ach	Acetylcholine
AIM	Automatic Identification of Markers
AIS	American Spinal Injury Association Impairment Scale
Ca ²⁺	Calcium
CAD	Computer-Aided Design
CE	Contractile Element
CE-IST	Ethics Commission of the Instituto Superior Técnico
CoP	Center of Pressure
DE	Damping Element
GRF	Ground Reaction Forces
GRM	Ground Reaction Moments
FEM	Finite Element Method
HAT	Head-Arms-Trunk
MTU	Muscle-Tendon Unit
MUBODYNA	MULTiBOdy DYNAMics
NS	Neural Signal

PA6	Polyamide 6
PE	Parallel Elastic Element
PVC	Polyvinyl Chloride
QUEST	Quebec User Evaluation of Satisfaction with Assistive Technology
RoM	Range of Motion
SCI	Spinal Cord Injury
SE	Series Elastic Element
sEMG	Surface Electromyography
SF-36	36-Item Short Form Survey
UNICEF	United Nations Children's Fund
WHO	World Health Organization

LIST OF SYMBOLS

The human body can be sectioned into three cardinal planes, namely frontal, sagittal, and transverse planes. When describing the position of a body segment with respect to another on each of these planes, different directional terms are utilized. In this work, the following terminology is adopted: anterior and posterior, medial and lateral, and superior and inferior, which correspond to the anteroposterior (x -direction), mediolateral (y -direction) and superoinferior (z -direction) directions, respectively.

Chapter 2

The general nomenclature used in section 2.4 is listed below. Specific variables and parameters utilized only in a particular formulation are locally described.

Latin Symbols

Symbol	Unit (SI)	Description
c	-	Damping parameter
f_x	N	Tangential ground reaction force in the anteroposterior direction
f_y	N	Tangential ground reaction force in the mediolateral direction
f_z	N	Normal ground reaction force
k	N/m	Stiffness parameter
v_0	m/s	Threshold velocity, tolerance velocity to smooth friction transition
v_x	m/s	Relative velocity in the anteroposterior direction
v_y	m/s	Relative velocity in the mediolateral direction
xyz	-	Global coordinate system

Greek Symbols

Symbol	Unit (SI)	Description
δ	m	Relative penetration or deformation

$\dot{\delta}$	m/s	Relative normal contact velocity
μ	-	Friction coefficient
μ_d	-	Dynamic friction coefficient
μ_s	-	Static friction coefficient

Subscripts

Symbol	Description
0	Initial condition
max	Relative to the maximum value of the corresponding variable
x	Relative to anteroposterior direction
y	Relative to mediolateral direction
z	Relative to superoinferior direction

Superscripts

Symbol	Description
m	Nonlinear exponent factor
n	Nonlinear exponent factor

Operators

Symbol	Description
($\cdot$)	First derivative with respect to time

Chapter 3

Latin Symbols

Symbol	Unit (SI)	Description
a	rad	Semi-axis of the ellipse
$\mathbf{a}_k$	-	Generic vector $\mathbf{a}$ defined in body k
$\mathbf{A}_k$	-	Transformation matrix of body k

b	rad	Semi-axis of the ellipse
$\mathbf{b}_k$	-	Generic vector $\mathbf{b}$ defined in body k
$\mathbf{b}_{j,p}$	-	Generic vector $\mathbf{b}$ defined in body k projected onto a plane p
$\mathbf{B}_h$	-	Transformation matrix of joint h
c	-	Coefficients of the polynomial
$\mathbf{c}^*(t)$	m	Experimental data containing the x , y , and z coordinates of the guided point G
$\mathbf{d}_{AB}$	m	Distance vector between points A and B
$\mathbf{d}$	m	Position vector connecting point P_i on body i to point P_j on body j or massless link vector
$\mathbf{D}$	-	Jacobian matrix of the constraint equations
e_0, e_1, e_2, e_3	-	Euler parameters
$e_k^*(t)$	-	Experimental data containing the Euler parameters to guide
f	N	Force magnitude
$\mathbf{f}$	N	Vector of external forces acting on a body
G	m	Magnitude of vector $\mathbf{r}_B$
$\mathbf{G}$	-	Transformation matrix in terms of the Euler parameters
$\mathbf{g}$	N, N·m	Vector of generalized external forces and gyroscopic moments
$\mathbf{g}^c$	N, N·m	Vector of reaction forces and moments on the kinematic joints
I	kg·m ²	Moment of inertia
$\mathbf{I}$	-	Identity matrix
j_h	N·m·s	Damping coefficient of a generic rotational joint h
l	-	Length parameter of the polynomial approach
l_{ml}	m	Length of the massless link
$\mathbf{l}$	m	Moment lever arm
$\mathbf{J}$	kg·m ²	Inertia tensor
m	kg	mass
$\mathbf{M}$	kg, kg·m ²	Global mass matrix
$m_{pe,h}$	N·m	Maximum moment applied to restrict the motion of a generic rotational joint h
$\mathbf{m}$	N·m	Moment vector
$\mathbf{m}_h^d$	N·m	Joint dissipative moment vector of a generic rotational joint h

$\mathbf{m}_h^{\text{mr}}$	N·m	Joint motion-restricting moment vector of a generic rotational joint h
$\mathbf{m}_h^{\text{r}}$	N·m	Joint resistance moment vector of a generic rotational joint h
N	-	Number of bodies
$\mathbf{n}$	N·m	Vector of external moments acting on a body
$\mathbf{n}_{CC}$	-	Unit vector normal to the surface of the circumduction cone
O_k	-	Center of mass of body k
$\mathbf{p}$	-	Euler parameters vector
$\mathbf{q}$	-	Vector of generalized coordinates
$\mathbf{R}$	-	Transformation matrix for circumduction cone's parameterization
$\mathbf{r}$	m	Arbitrary position vector for circumduction cone's parameterization
$\mathbf{r}_B$	m	Position vector for circumduction cone's parameterization at point B
$\mathbf{r}_k$	m	Position vector of the center of mass of body k in global coordinates
$\mathbf{r}_k^P, \mathbf{r}_k^G$	m	Global position vector of point P or G located on body k
$\mathbf{s}_k^P, \mathbf{s}_k^G$	m	Global position vector of point P or G located on body k with respect to local coordinates
$\mathbf{s}_k$	m	Vector placed on the joint axis belonging to body k
t	s	Time variable
$\mathbf{t}_G$	m	Vector tangent to the cone's surface along its generating line
$\mathbf{t}_\psi$	m	Vector tangent to the cone's surface along its perimeter
$\mathbf{t}$	-	Vector tangent to the cone's surface
$\mathbf{u}$	-	General vector
$\mathbf{u}_{\text{r},h}$	-	Unit vector defined using the moving body's local reference frame
$\mathbf{u}_{\text{r},h,\xi}$	-	Local ξ component of the unit vector $\mathbf{u}_{\text{r},h}$
$\mathbf{u}_{\text{r},h,\eta}$	-	Local η component of the unit vector $\mathbf{u}_{\text{r},h}$
$\mathbf{u}_{\text{r},h,\zeta}$	-	Local ζ component of the unit vector $\mathbf{u}_{\text{r},h}$
$\mathbf{u}_{\xi,h}$	-	Unit vector defining the ξ axis of joint h local reference frame
$\mathbf{u}_{\eta,h}$	-	Unit vector defining the η axis of joint h local reference frame
$\mathbf{u}_{\zeta,h}$	-	Unit vector defining the ζ axis of joint h local reference frame
$\mathbf{v}$	m/s, rad/s	Vector containing the system velocities
$\mathbf{v}_{\text{r}}$	m	Arbitrary vector for circumduction cone's parameterization
$\dot{\mathbf{v}}$	m/s ² , rad/s ²	Vector containing the system accelerations

$\mathbf{y}$	m, m/s, rad/s	Auxiliary vector containing the system velocities and positions
$\dot{\mathbf{y}}$	m/s, s ¹ , m/s ² , rad/s ²	Auxiliary vector containing the system accelerations and velocities
xyz	-	Global coordinate system

Greek Symbols

Symbol	Unit (SI)	Description
α	-	Baumgarte stabilization coefficient
β	-	Baumgarte stabilization coefficient
γ	-	Right-hand side vector of the acceleration constraint equations
ε	rad	Angle of the talocrural joint axis in the transverse plane
θ	rad	Angle of the talocalcaneal joint axis in the sagittal plane
$\theta^*(t)$	rad	Angle between the $\mathbf{a}_i$ and $\mathbf{b}_j$ vectors calculated using experimental data
κ	rad	Relative angular motion between the moving body and the limits of the circumduction cone
λ	-	Lagrange multipliers vector
$\mathbf{v}$	-	Right-hand side vector of the velocity constraint equations
ρ	rad	Angle of the talocalcaneal joint axis in the transverse plane
σ_h	rad	Latitude of a generic rotational joint h
$\sigma_{h,\max}$	rad	Maximum latitude of a generic rotational joint h
$\Delta\sigma_h$	rad	Difference between the passive and active range of motion of a generic rotational joint h
τ	rad	Angle of the talocrural joint axis in the frontal plane
φ	rad	Angle of the modified universal joint between the $\mathbf{a}_i$ and $\mathbf{u}_{r,h,p}$ vectors
$\varphi^*(t)$	rad	Angle between the $\mathbf{a}_i$ and $\mathbf{d}_p$ vectors calculated using experimental data
$\phi^*(t)$	rad	Angle between the $\mathbf{a}_i$ and $\mathbf{b}_{j,p}$ vectors calculated using experimental data
Φ	-	Position constraint equations vector
$\dot{\Phi}$	-	Velocity constraint equations vector
$\ddot{\Phi}$	-	Acceleration constraint equations vector
ψ_h	rad	Longitude of a generic rotational joint h
ω	rad/s	Angular velocity vector
$\dot{\omega}$	rad/s ²	Angular acceleration vector

$\xi\eta\zeta$	-	Body fixed coordinate system
$\xi_h\eta_h\zeta_h$	m	Joint local coordinate system

Subscripts

Symbol	Description
0	Initial condition or initial configuration or initial coordinates
A	Relative to point A
B	Relative to point B
C	Relative to point C
G	Relative to point G
h	Relative to a generic rotational joint h
i	Relative to body i
j	Relative to body j
k	Relative to body k
ml	Relative to the massless link
n	Degree of the polynomial curve
pe	Penalty
p	Projected
re	Real angle
t	Relative to time instant t

Superscripts

Symbol	Description
d	Relative to the dissipative moment
k	Parameter that allows to identify the polynomial curve
mr	Relative to the motion-restricting moment
r	Relative to the resistance moments
P	Generic point P
u_m	Relative to the modified universal joint
*	Relative to experimental data

Operators

Symbol	Description
$()^T$	Matrix or vector transpose
$(')$	Components of a vector in a body-fixed coordinate system
$('')$	Components of a vector in the joint's coordinate system
$(\dot{ })$	First derivative with respect to time
$(\ddot{ })$	Second derivative with respect to time
$(\sim)$	Skew-symmetric matrix of a vector
$(\ \)$	Vector norm

Chapter 4

Latin Symbols

Symbol	Unit (SI)	Description
a^m	-	Muscle activation
$\mathbf{a}_i$	-	Vector utilized to define driving constraint to guide the joint angle
$\mathbf{b}_j$	-	Vector utilized to define driving constraint to guide the joint angle
$\mathbf{D}$	-	Jacobian matrix of the constraint equations
e_0, e_1, e_2, e_3	-	Euler parameters
f^f	N	Fiber force magnitude
f^m	N	Muscle force magnitude
f_0^m	N	Maximum isometric muscle force magnitude
f_{CE}^m	N	Contractile element force magnitude
f_l^m	N	Force-length relation magnitude
f_{PE}^m	N	Parallel elastic element force magnitude
f_v^m	N	Force-velocity relation magnitude
f^t	N	Tendon force magnitude
f^{mtu}	N	Muscle-tendon unit force magnitude
$\mathbf{f}^{mtu}$	N	Muscle-tendon unit force vector

$\mathbf{f}$	N	Vector of external forces acting on a body
$\mathbf{f}_{CE}^{mtu}$	N	Contractile element force projected onto the line of action of the tendon
$\mathbf{f}_{PE}^{mtu}$	N	Passive element force projected onto the line of action of the tendon
$\mathbf{f}_{eq}$	-	Equality condition
$f_i(\mathbf{x}), f_j(\mathbf{x})$	-	Constraint equations to which the control variables are subjected
$\mathbf{g}$	N, N·m	Vector of generalized external forces and gyroscopic moments
$\mathbf{g}^{ext}$	N, N·m	Vector of the remaining external generalized forces and moments
$\mathbf{g}^{mtu}$	N, N·m	Vector of generalized muscle-tendon unit forces and moments
$\hat{\mathbf{g}}_{CE}^{mtu}$	N, N·m	Vector of the generalized forces and moments of the available contractile element force projected onto the line of action of the tendon
$\mathbf{g}_{PE}^{mtu}$	N, N·m	Vector of generalized forces and moments of the passive element projected onto the line of action of the tendon
I	kg·m ²	Moment of inertia
l^m	m	Muscle length
l_0^m	m	Optimal muscle length
l^{mtu}	m	Muscle-tendon unit length
l^t	m	Tendon length
l^w	m	Muscle width
$\mathbf{M}$	kg, kg·m ²	Global mass matrix
n_a	-	Number of muscle activations
n_b	-	Number of bodies
n_c	-	Number of constraint equations
n_{dv}	-	Number of design variables
n_{ec}	-	Number of equality constraint equations
$n_{f^{mtu}}$	-	Number of forces exerted on the application points
n_{mtu}	-	Number of muscle-tendon units
n_m	-	Number of muscles
n_p	-	Total number of points defining the muscle-tendon unit
n_{tc}	-	Total number of constraint equations
n_u	-	Number of direction unit vectors
n_{vp}	-	Number of via-points utilized to define the muscle-tendon unit
n_λ	-	Number of Lagrange multipliers

$\mathbf{n}$	N·m	Vector of external moments acting on a body
$\mathbf{r}_k^P$	m	Global position vector of point P located on body k
$\mathbf{u}_d$	-	Direction unit vector
v^m	m/s	Muscle velocity
v_0^m	m/s	Maximum contractile velocity
v^{mtu}	m/s	Muscle-tendon unit velocity
v^t	m/s	Tendon velocity
$\dot{\mathbf{v}}$	m/s ² , rad/s ²	Vector containing the system accelerations
x_i^{lower}	-	Lower bound side constraints for the optimization
x_i^{upper}	-	Upper bound side constraints for the optimization
$\mathbf{x}$	-	Vector of the design variables x
xyz	-	Global coordinate system

Greek Symbols

Symbol	Unit (SI)	Description
α	rad	Pennation angle
α_0	rad	Optimal pennation angle
$\dot{\alpha}$	rad/s	Pennation angular velocity
ε	-	User-specified tolerance
$\theta^*(t)$	rad	Angle between the $\mathbf{a}_i$ and $\mathbf{b}_j$ vectors to guide the revolute joint
λ	-	Lagrange multipliers vector
λ^R	-	Vector of the Lagrange multipliers associated with the joint constraints and the rigid body driving constraints
λ^*	-	Vector of the Lagrange multipliers associated with the rotational driving constraints of the joints spanned by the muscles
$\bar{\sigma}$	N/m ²	Specific muscle strength
χ	N, N·m	Vector containing the vectors of the generalized forces and moments of the available contractile element force projected onto the line of action of the tendon of each muscle-tendon unit
$\mathfrak{T}_0(\mathbf{x})$	-	Cost function to be minimized
$\xi\eta\zeta$	-	Body fixed coordinate system

Subscripts

Symbol	Description
CE	Relative to the contractile element
k	Relative to body k
PE	Relative to the parallel elastic element
vp	Relative to the via-point

Superscripts

Symbol	Description
m	Relative to the muscle
mtu	Relative to the muscle-tendon unit
t	Relative to the tendon

Operators

Symbol	Description
$()$	First derivative with respect to time
∇	Gradient of a function
$\wedge$	Relative to the available force

Chapter 5

Latin Symbols

Symbol	Unit (SI)	Description
$\mathbf{A}_k$	-	Transformation matrix of body k
$\mathbf{A}_{MC}$	-	Transformation matrix of the marker cluster plate
$\mathbf{D}$	-	Jacobian matrix of the constraint equations
e_0, e_1, e_2, e_3	-	Euler parameters
$\mathbf{G}$	-	Transformation matrix in terms of the Euler parameters
I	kg·m ²	Moment of inertia

$\mathbf{I}$	-	Identity matrix
l_b	m	Length of body b
m_b	kg	Mass of body b
$\mathbf{p}_k$	-	Vector containing three Euler parameters of body k
$\mathbf{q}$	-	Vector of generalized coordinates
$\mathbf{q}^c$	-	Vector containing the corrected positions
$\mathbf{q}^u$	-	Vector containing the uncorrected positions
$\delta\mathbf{q}$	-	Set of corrections that eliminates the position constraints violation
$\mathbf{r}^K$	m	Position vector of point K in global coordinates
$\mathbf{r}_k$	m	Position vector of the center of mass of body k in global coordinates
$\mathbf{r}_k^P$	m	Global position vector of point P located on body k
$\mathbf{s}_k^P$	m	Global position vector of point P located on body k with respect to local coordinates
$\mathbf{s}_{MC}^{K,M}$	m	Global position vector connecting marker K to marker M located on the marker plate MC with respect to local coordinates
$\mathbf{s}_k$	m	Vector placed on the joint axis belonging to body k
$\mathbf{U}$	-	Matrix containing the position, Euler parameters, linear velocities and angular velocity of all bodies of the multibody model
$\mathbf{v}_{aux}$	-	Auxiliary vector
$\mathbf{v}$	m/s, rad/s	Vector containing the system velocities
$\dot{\mathbf{v}}$	m/s ² , rad/s ²	Vector containing the system accelerations
$\mathbf{v}^c$	-	Vector containing the corrected velocities
$\mathbf{v}^u$	-	Vector containing the uncorrected velocities
$\delta\mathbf{v}$	-	Set of corrections that eliminates the velocity constraints violation
xyz	-	Global coordinate system

Greek Symbols

Symbol	Unit (SI)	Description
γ	-	Right-hand side vector of the acceleration constraint equations
λ	-	Lagrange multipliers vector
$\mathbf{v}$	-	Right-hand side vector of the velocity constraint equations
Φ	-	Position constraint equations vector

$\dot{\Phi}$	-	Velocity constraint equations vector
$\ddot{\Phi}$	-	Acceleration constraint equations vector
ω	rad/s	Angular velocity vector
$\xi\eta\zeta$	-	Body fixed coordinate system

Subscripts

Symbol	Description
A	Relative to point A
B	Relative to point B
C	Relative to point C
e	Relative to the Euler parameter e
i	Relative to body i
j	Relative to body j
k	Relative to body k
l	Relative to the left side
MC	Relative to the marker cluster plate
r	Relative to the right side

Superscripts

Symbol	Description
bf	Relative to the body-follower joint
A	Relative to marker A
B	Relative to marker B
C	Relative to marker C
c	Relative to corrected positions or velocities
P	Relative to point P
u	Relative to uncorrected positions or velocities

Operators

Symbol	Description
$(\cdot)^T$	Matrix or vector transpose
$(\dot{\cdot})$	First derivative with respect to time
$(\ddot{\cdot})$	Second derivative with respect to time
$(\sim)$	Skew-symmetric matrix of a vector

Chapter 6

Latin Symbols

Symbol	Unit (SI)	Description
$\mathbf{a}_i, \mathbf{b}_j, \mathbf{c}_i, \mathbf{d}_j, \mathbf{e}_i, \mathbf{f}_j$	-	Vectors utilized to define the fixed joint
c_r	-	Coefficient of restitution
d	m	Distance from the center of the sphere to the plane
$\mathbf{d}$	m	Vector from the center of the sphere to the plane
$\mathbf{D}$	-	Jacobian matrix of the constraint equations
E_k	Pa	Young's modulus of body k
f_c	N	Magnitude of the Coulomb friction
f_n	N	Normal contact force magnitude
$\mathbf{f}_n$	N	Normal contact force vector
$\mathbf{f}_t$	N	Tangential contact force vector
I	$\text{kg}\cdot\text{m}^2$	Moment of inertia
$\mathbf{I}$	-	Identity matrix
K	$\text{N}/\text{m}^{1.5}$	Generalized contact stiffness
$\mathbf{M}_k$	m	Vector containing the coordinates of the marker k
n	-	Hertzian nonlinear exponent
$\mathbf{n}_j$	-	Unit vector normal to the plane
R	m	Radius of the sphere
$\mathbf{r}_k$	m	Position vector of the center of mass of body k in global coordinates

$\mathbf{r}_k^P$	m	Global position vector of point P located on body k
$\mathbf{s}_k^P$	m	Global position vector of point P located on body k with respect to local coordinates
$\mathbf{t}$	-	Tangential direction of the relative velocity associated with the contacting surfaces
$\mathbf{U}$	-	Matrix containing the position, Euler parameters, linear velocities and angular velocity of all bodies of the multibody model
v_1	m/s	Threshold for the velocity
v_t	m/s	Magnitude of the relative tangential velocity
$\mathbf{v}_n$	m/s	Relative normal velocity of the contact points
$\mathbf{v}_t$	m/s	Relative tangential velocity of the contact points
$\mathbf{v}_{aux}$	-	Auxiliary vector
xyz	-	Global coordinate system

Greek Symbols

Symbol	Unit (SI)	Description
δ	m	Penetration depth
$\dot{\delta}$	m/s	Penetration velocity
$\dot{\delta}^{(-)}$	m/s	Initial contact velocity
γ	-	Right-hand side vector of the acceleration constraint equations
μ_k	-	Kinetic coefficient of friction
Φ	-	Position constraint equations vector
$\dot{\Phi}$	-	Velocity constraint equations vector
$\ddot{\Phi}$	-	Acceleration constraint equations vector
ω	rad/s	Angular velocity vector
$\dot{\omega}$	rad/s ²	Angular acceleration vector
σ_k	Pa ¹	Material property of body k
ν_k	-	Poisson's ratio of body k
χ	Ns/m ^{1.5}	Hysteresis damping factor
$\xi\eta\zeta$	-	Body fixed coordinate system

Subscripts

Symbol	Description
i	Relative to body i (sphere)
j	Relative to body j (plane)
k	Relative to body k

Superscripts

Symbol	Description
f	Relative to the fixed joint
C	Relative to point C of the center of the sphere
G	Relative to point G of the plane
P	Relative to point P
Q	Relative to the contact point

Operators

Symbol	Description
0	Initial condition or initial configuration or initial coordinates
$(\cdot)^T$	Matrix or vector transpose
$(\dot{\cdot})$	First derivative with respect to time
$(\ddot{\cdot})$	Second derivative with respect to time
$(\tilde{\cdot})$	Skew-symmetric matrix of a vector

Appendixes

Latin Symbols

Symbol	Unit (SI)	Description
a^m	-	Muscle activation
A_k	-	Transformation matrix of body k
D	-	Jacobian matrix of the constraint equations

f_0^m	N	Maximum isometric muscle force magnitude
f_{CE}^m	N	Contractile element force magnitude
f_l^m	N	Force-length relation magnitude
f_{PE}^m	N	Parallel elastic element force magnitude
f_v^m	N	Force-velocity relation magnitude
f^{mtu}	N	Muscle-tendon unit force magnitude
$\mathbf{f}^{mtu}$	N	Muscle-tendon unit force vector
$\mathbf{f}$	N	Vector of external forces acting on a body
h	m	Height
I	kg·m ²	Moment of inertia
l	m	Length
l^m	m	Muscle length
l_0^m	m	Optimal muscle length
l^t	m	Tendon length
l_f	m	Foot length
m^{mtu}	N·m	Muscle-tendon unit moment
ma^{mtu}	m	Moment arm of the muscle-tendon unit
m	kg	Mass
$\mathbf{n}$	N·m	Vector of external moments acting on a body
r	m	Radius of gyration
$\mathbf{r}_k$	m	Position vector of the center of mass of body k in global coordinates
$\mathbf{r}_k^P$	m	Global position vector of point P located on body k
R_{el}	m	Ellipsoid radius
$\mathbf{R}_{el}$	m	Matrix containing the ellipsoid radii
$\mathbf{s}_k^P$	m	Global position vector of point P located on body k with respect to local coordinates
$\mathbf{s}_k$	m	Vector placed on the joint axis belonging to body k
$\mathbf{u}_d$	-	Direction unit vector
v_0^m	m/s	Maximum contractile velocity
xyz	-	Global coordinate system

Greek Symbols

Symbol	Unit (SI)	Description
α	rad	Pennation angle
γ	-	Right-hand side vector of the acceleration constraint equations
κ	-	Scaling factor
Φ	-	Position constraint equations vector
$\dot{\Phi}$	-	Velocity constraint equations vector
$\ddot{\Phi}$	-	Acceleration constraint equations vector
ω	rad/s	Angular velocity vector
$\dot{\omega}$	rad/s ²	Angular acceleration vector
$\xi\eta\zeta$	-	Body fixed coordinate system

Subscripts

Symbol	Description
CE	Relative to the contractile element
$e/$	Relative to the ellipsoid
i	Relative to body i
j	Relative to body j
k	Relative to body k
PE	Relative to the parallel elastic element
Q	Relative to data taken from Quental (2013)
Rj	Relative to data taken from Rajagopal et al. (2016)
vp	Relative to the via-point

Superscripts

Symbol	Description
b	Relative to the body
$e/$	Relative to the ellipsoid
m	Relative to the muscle
mtu	Relative to the muscle-tendon unit

P	Generic point P
Q	Generic point Q
t	Relative to the tendon

Operators

Symbol	Description
$()^T$	Matrix or vector transpose
$(')$	Components of a vector in a body-fixed coordinate system
$('')$	Components of a vector in the joint's coordinate system
$(\dot{ })$	First derivative with respect to time
$(\ddot{ })$	Second derivative with respect to time
$(\tilde{ })$	Skew-symmetric matrix of a vector

"Happiness can be found, even in the darkest of times, if one only remembers to turn on the light."

J.K. Rowling, Harry Potter and the Prisoner of Azkaban

1. INTRODUCTION

The World Health Organization (WHO) and the United Nations Children's Fund (UNICEF) estimate that nowadays more than 2.5 billion people worldwide use one or more assistive devices, and this number is expected to rise to 3.5 billion in 2050. The use of mobility assistive device, such as crutches, walkers, wheelchairs and canes, presents functional benefits for disabled subjects, as they improve independence, enable the participation in social activities and reduce the need for hospitalization, leading to lower health costs. However, the incorrect and repetitive use of assistive devices may lead to the onset of secondary health conditions. Thus, there is a growing tendency to use biomechanical models to study device-assisted locomotion. This chapter provides a general overview of the motivation and relevance of this work, as well as the scope and associated objectives. The organization of the document, including a description of the content of each chapter, is provided, followed by the contributions of the investigation.

1.1. Motivation and Relevance

The 2022 global report on assistive technology of the World Health Organization (WHO) and the United Nations Children's Fund (UNICEF) estimates that more than 2.5 billion people globally require the use of one or more assistive devices, and this number is expected to rise to 3.5 billion in 2050 (World Health Organization & United Nations Children's Fund - UNICEF, 2022). Commonly, an assistive device is defined as any item, piece of equipment or product, whether acquired commercially, modified, or customized, that is utilized to maintain or improve the functional capabilities of subjects (Carver et al., 2016; World Health Organization, 2016). The elderly, people with disability, noncommunicable diseases or mental health conditions, and people suffering from progressive functional decline are among those most in need of these devices. They are utilized to compensate for an impairment or loss of intrinsic capacity, reduce the consequences of gradual functional decline and help minimize the need for caregivers. The use of assistive devices presents crucial functional benefits for subjects with permanent or temporary disability, as they not only improve independence, but also enable and enhance the

participation in social activities, including school and work, and reduce the need for hospitalization, leading to lower health and welfare costs. Without the possibility of using these devices, subjects are at a higher risk of social exclusion, of falling into poverty, or of depending on their family and society to a greater extent. Therefore, it is evident that the positive impact of assistive devices goes far beyond improving the health and well-being of individual users. Assistive devices can help alleviate disability in six functional categories, namely, hearing, vision, mobility, communication, self-care, and cognition, with mobility disability being the second most common functional difficulty (Carver et al., 2016; World Health Organization, 2016; World Health Organization., 2021).

Mobility disability can be described as a difficulty in walking or an inability to ambulate without great difficulty or assistance. It encompasses the surrounding environment of the subject and his/her ability of adapting to it (C. J. Brown & Flood, 2013; Cardona et al., 2020; Simonsick et al., 2008). Mobility disability has been associated with increased fall, hospitalization, and mortality risks, as well as decreased quality of life and poor psychosocial health (Freiberger et al., 2020). A variety of health conditions and pathologies can affect key aspects of mobility, including balance, control, and stability, leading to disability (Cardona et al., 2020). The etiology of these health conditions and pathologies can broadly be classified into neurological, musculoskeletal, and cognitive. Among neurological causes, stroke, spinal cord injury, cerebral palsy, muscular dystrophy, poliomyelitis, spina bifida, including myelomeningocele, and multiple sclerosis commonly affect pediatric and adult populations. Musculoskeletal conditions include arthritis, osteogenesis imperfecta, and osteoporosis, and cognitive conditions involve, for instance, the Alzheimer's disease (Cardona et al., 2020; Cook et al., 2019). Amputation, diabetes, obesity, and cardiorespiratory conditions can also cause mobility disability (Cook et al., 2019). Depending on their level and type of disability, subjects are prescribed with the most appropriate mobility assistive device. In this section, four mobility assistive devices are approached, namely crutches, walkers, canes, and wheelchairs.

Crutches are utilized as a mean of locomotion by patients with a variety of pathologies, providing them with a good level of mobility and flexibility. They are utilized to increase patients' balance and base of support, and to partially or fully unload the lower limbs by transferring the body weight to the upper extremities. These assistive devices can be classified into axillary, forearm, and platform crutches. Axillary crutches, also referred to as standard or regular crutches, are made of aluminum or lightweight wood. Each crutch is made up of two upright pieces joined together at the top by an axillary bar, at the middle by a handgrip and at the distal end by one vertical piece with a rubber tip (see Figure 1.1a). Forearm crutches, also called Lofstrand or Canadian crutches, consist of a single support with a handgrip and a forearm cuff (see Figure 1.1b). This type of crutches is usually made of aluminum with a rubber tip, and

the patients' weight is almost exclusively borne by the handgrip, requiring great upper body strength and coordination. Axillary crutches provide more stability than forearm crutches since the latter lacks axillary control. The absence of the axillary portion on forearm crutches eliminates the danger of axillary damage. Platform crutches are recommended for patients who cannot grip the handgrips of axillary or forearm crutches or bear weight through their wrists or hands. These crutches have a platform at the top with a handgrip (see Figure 1.1c) (Dreeben-Irimia, 2010; Johansson & Chinworth, 2018; Lindh et al., 2009).

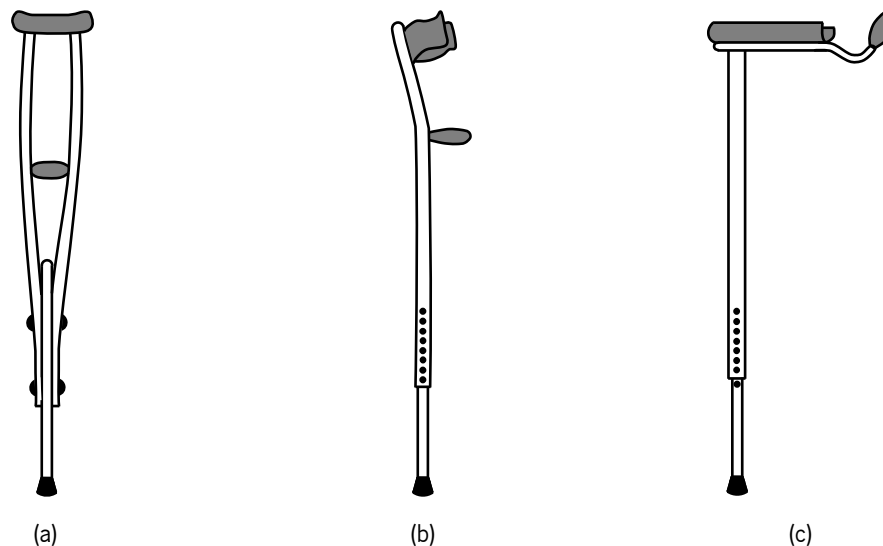


Figure 1.1 – Types of crutches. (a) Axillary crutches. (b) Forearm crutches. (c) Platform crutches.

Walkers improve balance and partially or fully unload injured lower extremities by supporting the body weight through the patients' arms. These assistive devices provide four points of contact with the floor and a wide base of support and stability. However, in small or confined areas and stairs, walkers may be difficult and dangerous to use (Acello & Hegner, 2015; Johansson & Chinworth, 2018; Lindh et al., 2009). Walkers can be found in many designs, and, in all of them, the walker should be wide enough to allow the patient to walk into it (Acello & Hegner, 2015). An illustration of walker types is presented in Figure 1.2, namely standard, rolling, and rollator walkers. Standard walkers, also known as pickup walkers, do not have wheels and provide the greatest amount of stability (see Figure 1.2a). Compared with other walkers, the standard walker demands more energy expenditure, reduces the gait speed, and interferes with the normal gait pattern. Rolling walkers, also designated by wheeled walkers, require less energy expenditure than the standard type and enable a more conventional gait speed (see Figure 1.2b). This walker type is a better option for patients who primarily need balance. The greater the number of wheels, the greater the mobility and the lower the stability. The rollator walker typically has four wheels and a built-in seat, and many of them also have a basket at the front (see Figure 1.2c). This walker design allows the patient to sit and rest regularly (Johansson & Chinworth, 2018; Lindh et al., 2009).

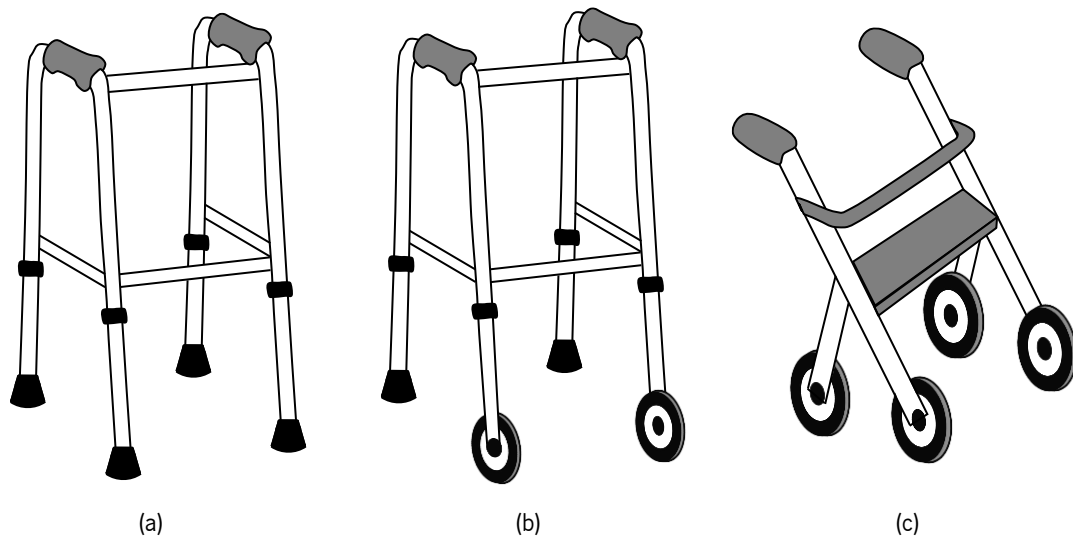


Figure 1.2 – Types of walkers. (a) Standard walker. (b) Rolling walker. (c) Rollator walker.

Wheelchairs allow subjects with severe ambulation conditions or no ability to ambulate at all to move and are fundamental to their independence. There are two types of wheelchairs, manual and motorized or powered (Harvey, 2008; Lindh et al., 2009; Suryadevara & Mukhopadhyay, 2020). The type of wheelchair prescribed to a subject depends on his/her pathological level of impairment (Harvey, 2008). A manual wheelchair does not have a power source and it is propelled by the user or by another individual (Bouck, 2017). It consists of a seat, footrests, and wheels at the back and front, as represented in Figure 1.3. The handrims of these assistive devices have a diameter that is slightly smaller than that of the back wheels, and most manual wheelchairs have push handles at the top of the back to enable manual propulsion by other individuals. The manual wheelchair propulsion cycle can be divided into two phases, namely contact or push, and recovery phases. In the push phase, mechanical power is delivered to the wheelchair via hand contact with the handrim, whilst in the recovery phase, the hand is repositioned in preparation for the next cycle (Kwarciak et al., 2009).

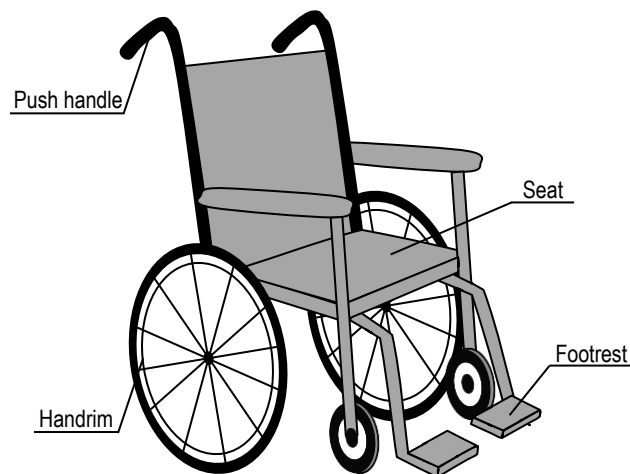


Figure 1.3 – Schematic representation of a manual wheelchair.

Canes can be used by patients with one good arm only and are primarily utilized to improve balance and stability, to widen the base of support and to decrease loads placed on the lower extremities. For an optimal reduction of the forces transmitted through the lower extremities, the cane should be held in the hand opposite to the injured lower extremity (Dreeben-Irimia, 2010; Johansson & Chinworth, 2018). Canes consist of a single upright piece adjustable or not in height, and, depending on their base, they can be classified into two main groups, namely standard or single-point, and quadruped or four-point canes (Johansson & Chinworth, 2018). Standard canes have a curved handle for gripping (see Figure 1.4a), and the most recent ones have a handgrip attached (see Figure 1.4b). This type of cane is utilized by patients with less severe walking conditions and that need little amount of support (Lindh et al., 2009). In turn, quadruped canes rest on a four-legged platform, and, due to the additional points of contact with the ground, they offer greater levels of stability and a wider base of support when compared with standard canes but provide a slower gait. They are utilized by patients with more severe walking difficulties. Quadruped canes can be classified into small-based and large-based, as observed in Figure 1.4c and Figure 1.4d, respectively (Dreeben-Irimia, 2010; Johansson & Chinworth, 2018; Lindh et al., 2009).

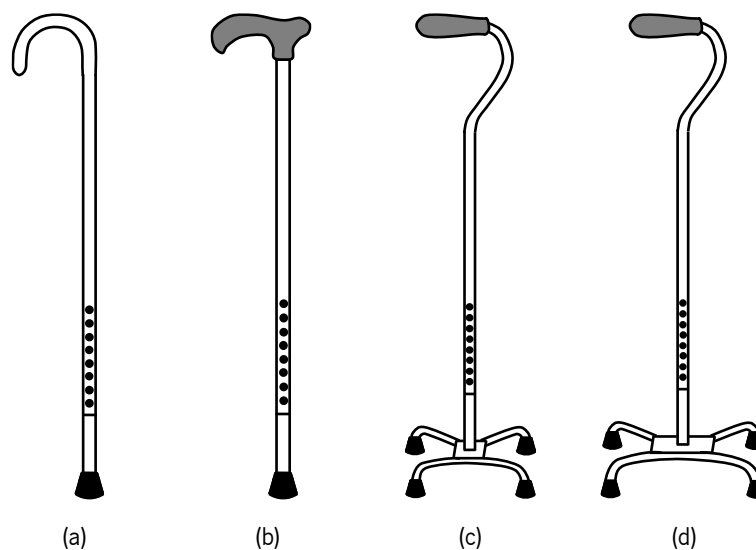


Figure 1.4 – Types of canes. (a) Standard cane. (b) Standard cane with handgrip. (c) Small-based quadruped cane. (d) Large-based quadruped cane.

Patients with mobility disabilities use crutches, walkers, wheelchairs, or canes to restore the mobility lost due to the disability, which allows them to regain some degree of independence (Carver et al., 2016). The use of these devices has a positive impact on the quality of life of patients at both psychological and physiological levels, including the improvement in cardiovascular, digestive, and respiratory functions (Holanda et al., 2017). An assistive device that is properly fitted to the patient allows for more comfortable locomotion and requires less energy expenditure. However, the incorrect, repetitive,

and prolonged use of mobility assistive devices can have harmful consequences for patients, including pain and discomfort, as their body weight is largely unloaded into the devices, imposing a considerable repetitive effort on the upper extremities, which are not adapted to weight-bearing tasks. This phenomenon leads to the appearance of secondary musculoskeletal, neurological, and vascular health conditions, such as glenohumeral and wrist tendinopathies, or peripheral nerve injuries, which cause morbidity and functional loss (Edelstein, 2019; Manocha et al., 2021). Thus, there is an urgent need to address this issue by understanding the biomechanics of device-assisted gait.

The biomechanics of motion discipline applies principles and laws of mechanics to analyze the movement of living beings. The study of the human movement using the multibody systems methodology is a challenging scientific field of investigation that has undergone vast developments over the last years, and it is extensively utilized in several engineering applications. Multibody systems methodologies are perhaps the most suitable tools for the biomechanical modelling and analysis of the human movement as they allow to noninvasively investigate the relation existing between the body motion and the internal joint loads in a variety of experimental settings. In this sense, numerous computational biomechanical models of the human body have been and continue to be developed in order to study and analyze the biomechanics of healthy and pathological human movement. The combination of these computational models with experimental information of the human motion provides estimates of biomechanical parameters, such as muscle or joint forces, that are not easily measured in experimental settings (Moissenet et al., 2017; I. Roupa et al., 2022; M. Silva et al., 2021; Tepe & Peterson, 2017). The validity of the predicted results relies on the development of realistic biomechanical models, including reliable modelling of anatomical segments, articulations, muscles, and body-environment interactions (e.g. foot-ground contact) (Flores & Lankarani, 2016). This knowledge helps to understand how mobility disabilities affect the human movement and provides promising options for the development of mobility assistive devices tailored to the needs of each subject, as well as type and level of pathology causing the disability.

Despite the existing investigation, the study of device-assisted locomotion has not become an established routine yet, and difficulties still exist in understanding how it may impact clinical intervention strategies and rehabilitation procedures, ultimately ensuring usefulness in real-world medical contexts. In addition, one of the most critical and challenging aspects when studying device-assisted locomotion is the interaction that occurs between the assistive device and the surrounding environment, namely the interaction between the device and the ground, and the interaction between the device and the user. Hence, this work aims to develop an advanced musculoskeletal model of the human movement within the framework of multibody system methodologies in order to study and understand device-assisted gait

with focus on mobility assistive devices. This knowledge may shed light on the biomechanical loads placed on the upper limbs and can guide the design of novel mobility assistive devices that improve the gait efficiency and also increase the end-user comfort. The successful accomplishment of this work is a step ahead in the improvement of the quality of life of disabled patients according with the Goal 3, Good Health and Well-Being, of the United Nations Sustainable Development Goals.

1.2. Scope and Objectives

The present work was developed under the mechanical engineering doctoral program of the University of Minho. This doctoral program aims at granting advanced education in the classical areas of mechanical engineering, namely mechanical project, metallurgy, and mechanics of materials, as well as on emergent areas of mechanical engineering, such as biomechanics, energy and environment, functionalized materials, and surface behavior. It is intended that the students develop research and experimental methodologies and competencies that allow the autonomous development, both individually or in teams, of research and development activities. These activities include state of the art knowledge, project planning, selection and application of research methods and procedures, and report results. The main aim of the program is to train highly qualified specialists and researchers capable of performing autonomous research, development, and innovation work in the area of mechanical engineering. The acquired competencies and culture will enhance the interaction between the university and the business community, contributing to the competitiveness and sustainability of the mechanical engineering sector.

The present study is a multidisciplinary work that combines mechanical and biomedical engineering to study device-assisted gait. Biomechanics of movement is the scientific field in which this project is involved, being one of the areas on which the mechanical engineering doctoral program aims at granting advanced education. Following the philosophy of the doctoral program, close cooperations with ORTHOS XXI, a European manufacturer of a variety of orthopedic and hospital equipment, and with *Centro de Reabilitação do Norte – Dr. Ferreira Alves*, a national and international reference center that responds to the health needs of rehabilitation, were established. The collaborations were critical for the successful achievement of this work and resulted in powerful interaction between the research conducted at the university, the industrial sector, and the clinical practice, enabling a closer-to-reality perspective.

In order to guarantee the success of a research project, it is of utmost importance to clearly define the main objective on which the investigation relies and for which it seeks a solution. Thus, the main objective of this work is to develop an advanced multibody musculoskeletal model of the human movement to study device-assisted gait. The approach is particularly targeted to a specific type of mobility

assistive devices, namely forearm crutches. The successful accomplishment of the main objective is based on several specific goals that are listed below, namely

- to develop a biomechanical multibody model with complete skeletal features, including human anatomical segments and articulations;
- to incorporate muscles in the biomechanical multibody model, including the contraction dynamics, the introduction into the equations of motion and the optimization procedures;
- to investigate the interactions that occur between the biomechanical multibody model and the ground, specifically the foot-ground contact;
- to incorporate mobility assistive devices in the developed biomechanical multibody model and specifically focus on the potential interactions generated between the device and the surrounding environment, i.e. device-model and device-ground contacts;
- to validate the proposed approach, that is, the biomechanical multibody model incorporated with a musculoskeletal system and mobility assistive devices;

Meeting the main objective and the specific goals defined for this work allows to overcome currently existing limitations related to the available solutions in the scientific field of biomechanics of movement and it is a step ahead in the state of the art of the application of musculoskeletal biomechanical models to the study of device-assisted gait. The developed methodologies are able to perform reliable analyses of device-assisted gait, and it is expected that, in the future, they serve as helpful tools both for the enhancement of clinical interventions and the design of assistive devices, ultimately improving the quality of life of patients. The procedures and results presented throughout this document demonstrate the accomplishment of the defined objectives for this work.

1.3. Organization of the Document

The present work focuses on the development and implementation of an advanced multibody musculoskeletal model of the human movement to study device-assisted gait. Due to its multidisciplinary nature, the work involves the interplay between a variety of fields of investigation, including multibody systems methodologies, skeletal muscle modeling, biomechanical modeling, driving constraints formulation and device-assisted gait analysis. Hence, this work is divided into seven chapters.

Chapter 1 comprises the description of the motivation and relevance of this work, and, in that context, the associated scope and objectives are listed. In the aftermath of this process, a general overview of the organization of this document is provided and the chapter ends with the indication of the contributions of the investigation.

In Chapter 2, a complete literature review of the main approaches associated with the biomechanical modeling of device-assisted locomotion is presented. Initially, a general description of the research methodology applied to identify and select the articles analyzed in the review is provided. Then, the chapter is divided according to the different fields of study involved in the present work. A general description and critical assessment of the current evidence on biomechanical modeling applied to device-assisted locomotion, targeting specifically crutches, walkers, canes, and wheelchairs, is presented. Then, a more focused description of crutch-assisted modeling procedures and how the interaction between these assistive devices and the ground or the human body is approached is offered. Different strategies currently employed to deal with the interaction between the human foot and the ground are also presented and critically discussed.

Chapter 3 involves the complete explanation of the multibody systems methodologies implemented and developed in this work. First, the adopted multibody dynamics formulation with Cartesian coordinates is revisited. The complete characterization of the methodology proposed to model the ankle joint complex, namely the modified universal joint, is presented. Then, a thorough explanation of the proposed methodology to restrict the range of motion of mechanical joints is provided. In addition, the driving constraints formulation developed to guide the degrees-of-freedom of the advanced multibody musculoskeletal model of the human movement is carefully described. The developed multibody methodologies are exploited in the dynamic modeling and simulation of three demonstrative examples of application, including a leg-foot model and a right lower limb model.

The Fourth Chapter includes a comprehensive description of the approaches utilized to model skeletal muscles. The chapter begins with an explanation of the underlying anatomical and physiological concepts associated with skeletal muscles, which involves a detailed understanding of the structures comprised within these tissues and constitutes the foundation for the modeling approaches employed in this work. The muscular contraction dynamics phenomenon is described, and the mathematical formulation utilized to incorporate the muscles into the advanced multibody model is provided. A Hill-type muscle model is utilized to mimic the contraction dynamics of the muscle tissue. The tendon, which connects muscles to bones, is assumed to be a rigid element. The process utilized to introduce the muscles into the equations of motion of the system and the optimization procedures are also described in detail. The chapter ends with two application examples to validate the implemented methodology and to provide realistic case scenarios.

Chapter 5 is entirely dedicated to the advanced multibody musculoskeletal model of the human movement. In this work, two three-dimensional biomechanical models are developed and implemented.

The biomechanical models share the same anthropometric parameters and the difference between them resides in the approach utilized to describe the shoulder joint complex. One model considers that the upper part of the trunk is connected to the arm via the glenohumeral joint only (simple model), while the other multibody model connects the two segments using a more detailed modeling of the shoulder joint complex (detailed model). A comprehensive description of the two models is provided, in which the segments and associated anthropometric properties, number and type of joints, as well as degrees-of-freedom are explained. The simple biomechanical model is utilized to analyze the experimental gait data of the human movement acquired at the Lisbon Biomechanics Laboratory. The adopted acquisition protocol, including the description of the utilized equipment and marker placement, and the data treatment procedures are approached in detail. The trajectory of the markers, ground reaction forces and surface electromyographic (sEMG) data were acquired. An important aspect to consider when acquiring experimental data of the human movement is that the processed kinematic data does not guarantee that the position and velocity constraints of the biomechanical models are fulfilled. Hence, in order to correct this issue, a kinematic consistency procedure is developed and applied to the model. Finally, the chapter ends with the discussion of one demonstrative example of application.

Chapter 6 provides the integration of all the methodologies and procedures developed in the previous chapters to study and analyze device-assisted gait, with specific focus on crutches. A collaboration with *Centro de Reabilitação do Norte – Dr. Ferreira Alves*, a specialized center that responds to the health needs of rehabilitation, was established in order to assess the pain perceptions associated with crutch use of patients suffering from chronic spinal cord injury. The objective was to recruit patients from the Spinal Cord Injury Rehabilitation Unit to answer a questionnaire, including, among other items, the determination of pain intensity, pain location, and utilized strategies to relieve pain. All the procedures undergone to establish the collaboration, including the submission of the study to the Ethics Committee of the *Centro Hospitalar de Vila Nova de Gaia/Espinho* and the followed protocol, are described in detail in this chapter. In addition, another collaboration was established with ORTHOS XXI, which is a European manufacturer of a wide of range of orthopedic and hospital equipment. ORTHOS XXI provided the crutches that were utilized in this work and also offered crucial assistance in aspects associated with the crutch development process, including the constituting materials, international standards that regulate crutch development, and computer aided design (CAD) modeling. The experimental protocol, procedures to introduce the crutches into the biomechanical model, as well as the approaches considered to handle the interactions between the crutch and the ground and between the crutch and the model are explained. The chapter ends with a case study, which incorporates and integrates the work developed in all chapters.

Finally, Chapter Seven summarizes the most relevant conclusions of the work. Selected lines of investigation are recommended for future developments in the field of device-assisted gait modeling.

1.4. Contributions of the Investigation

The work developed throughout the present doctoral thesis has mainly contributed to the development of the scientific field of biomechanics of motion. This PhD provides a three-dimensional biomechanical multibody model of the human movement incorporated with muscle modeling methodologies, mobility assistive devices and the corresponding interactions of the device with the surrounding environment (ground and model) to study device-assisted gait. Removing the assistive devices from the model, the evaluation of unassisted human gait can also be achieved.

In what concerns to the evaluation of the current state of the art on the analysis of device-assisted locomotion using computational biomechanical models, three complete and updated literature review papers have been written, being two of them published in a high impact factor scientific journal, and the other being under consideration in another journal. The comprehensive reviews comprise detailed analyses, discussion and summary of the key features of the computational strategies currently utilized to study device-assisted locomotion. The interested reader is referred to the list of publications resulting from the present PhD work that can be consulted at the end of this document.

Regarding the progress achieved within the framework of multibody systems methodologies, the present doctoral work resulted in the development of a novel kinematic joint model for the ankle joint complex of the human foot that considers the actual anatomy and movements of the talocrural and the talocalcaneal articulations. After a comprehensive analysis of the scientific literature, the reason for the development of the novel joint model is associated with the fact that most existing approaches do not consider a sufficiently accurate anatomical modeling of the ankle joint complex. Hence, the proposed approach uses a modified universal joint, which incorporates a massless link to mimic the actual function of the talus bone. Modeling the ankle joint complex as a modified universal joint allows a more realistic representation of the anatomy of the human foot. In addition, a novel methodology to restrict the range of motion (RoM) of mechanical joints has also been proposed. The main motivation behind this methodology is that mechanical joints are usually formulated as classical kinematic constraints such that there is no restriction of the RoM of the joint. Thus, additional restrictions to prevent the joints from performing unacceptable movements and to avoid unrealistic configurations of the connected bodies are formulated. The methodology proposes the use of joint resistance moments that are applied to the bodies connected by the joint to mimic the dissipative behavior of the materials constituent of joints and to

prevent unacceptable configurations of those bodies. Three papers associated with these contributions are published in scientific journals relevant to the respective areas of investigation. Finally, the present PhD work also contributes to the formulation of driving constraints utilized to guide the degree-of-freedom of the developed biomechanical multibody model. The driving constraints are expressed as functions of the time variable and are typically obtained experimentally by using an optoelectronic motion capture system. The formulation developed in this work to prescribe the experimental data to the biomechanical model considers driving constraints to guide the trajectory of a generic point, an arbitrary Euler parameter and the angle between two vectors. Although these driving constraint are utilized on the biomechanical model, they can be applied to guide the degrees-of-freedom of any model regardless of the scientific field of investigation. The formulation of the driving constraints was presented at an international conference.

The modeling of human skeletal muscles is approached in this work. The implemented concepts and methodology are based on previously published studies. However, the first application example lays the foundations for the publication of a collection of benchmark cases that will be a useful, imperative and truly important contribution for the international multibody dynamics community, as they will allow the validation of musculoskeletal models based on simple cases. The manuscripts is being prepared for submission. The biomechanical model with muscles has been presented in an international conference

Concerning the biomechanical multibody model, a novel type of joint has been developed. The proposed joint model, named body-follower joint, constrains the translational and orientational coordinates of a body j relative to the translational and orientational coordinates of a body i , thus removing the six degree-of-freedom of body j . The body-follower joint is applied in the radioulnar joint between the radius and the ulna, forcing the radius to follow the translation and orientation of the ulna. This procedure is carried out in order to consider these two anatomical segments as a unique body. Also, the utilized kinematic consistency procedure was based on a previously published direct correction approach. The approach has been adapted in order to be specifically utilized in the context of the experimental acquisition of the human movement and to deal with the elimination of the position and velocity constraints violation.

Finally, the questionnaire developed in collaboration with *Centro de Reabilitação do Norte* is a powerful tool for understanding the pain perceptions of patients while using mobility assistive devices. The collected information may identify adjustments that must be made to the device design and/or locomotion strategy that help improve the comfort and quality of life. The acquisition of experimental crutch-assisted gait data and the implementation of crutches into the biomechanical model are important contributions of this PhD. A specific type of joint was formulated, i.e. a fixed joint, to deal with the interface existing between the crutch and the model. In addition, the interaction between the crutch and the ground has been approached by a sphere-plane contact algorithm.

“Any piece of knowledge I acquire today has a value at this moment exactly proportional to my skill to deal with it. Tomorrow, when I know more, I recall that piece of knowledge and use it better.”

Mark Van Doren

2. LITERATURE REVIEW

Biomechanical models are useful tools for the analysis of the human body, as they allow to find the muscle and joint forces resulting from a certain movement. This knowledge is essential to help the development and improvement of mobility assistive devices tailored to each patients' needs. In this chapter, an overview of the current literature on the biomechanical modeling procedures utilized to analyze device-assisted locomotion is provided, which serves as the basis for the approaches developed in this work. Initially, the adopted research methodology to review the literature is described in detail. The application of the methodology is demonstrated in the assessment of the characteristics utilized in biomechanical models analyzing device-assisted locomotion and, more specifically, in the currently considered crutch modeling procedures. The solutions available in the scientific literature utilized to study the foot-ground interaction problem in human locomotion are also reviewed. The chapter ends with a summary and discussion of the compiled information.

2.1. Description of the Research Methodology

In order to review the literature on the topics of this work, a rigorous research methodology was adopted. The first step of the adopted research methodology is to establish the search strategy, which is defined using the Boolean operators AND/OR and combining a carefully selected list of keywords. The chosen keywords and their combination must allow to find the articles of interest on the topic of the review. An example of the search strategy utilized in section 2.2. and that was established to find studies including the use of biomechanical models combined with mobility assistive devices is given below.

SET 1: biomechanical OR skeletal OR musculoskeletal OR musculo-skeletal OR neuromusculoskeletal

SET 2: model*

SET 3: crutch* OR cane* OR walker* OR wheelchair* OR “assistive device” OR “assistive devices” OR “mobility aid” OR “mobility aids” OR “assisted walking”

Search strategy: SET 1 AND SET 2 AND SET 3

It is important to note that the asterisk is a frequently utilized wildcard symbol that expands a search by identifying words that share the same initial letters. It is particularly helpful when it is intended to retrieve complex variations of the root of the search term. For instance, in the above example, the term *model** is utilized, in which the root of the search term is *model*. By using the asterisk, all words including the term *model* are retrieved, such as *models*, *modeling*, *modelling*, *modeled* and *modelled*. In addition, the use of quotation marks allows to find two or more search terms as a whole, instead of the individual search terms. Searching with quotation marks finds results that include all the search terms in that specific order. Searching without quotation marks also retrieves results that include the search terms, but not necessarily in the searched order. For example, in the above search strategy, the quotation marks are utilized in “assistive device” to find the search terms exactly how they are written.

After the definition of the search strategy, the databases on where the defined list of keywords will be introduced must be selected. In this work, the search strategies defined for the topics included in sections 2.2., 2.3. and 2.4 were introduced into three electronic databases, namely PubMed, Web of Science and Scopus, and no restrictions on year of publication were considered. Independently of the considered electronic database, using only one database is not a suitable approach as its coverage may not be complete and it varies according to the research field. Thus, searching in more than one database is a good practice. The three databases chosen in this work are complementary to each other, and they were selected in order to guarantee appropriate coverage of the studies published in each topic to review. The field tags [Title/Abstract], [Topic] and [Article Title/Abstract/Keywords] were utilized to introduce the list of keywords on PubMed, Web of Science and Scopus, respectively. On the Web of Science database, the search strategy was carried out on all editions of the core collection. When introducing the search strategy into the electronic databases, the date on which this procedure is performed must be saved and reported. This procedure ensures reproducibility of the results and provides information about the currency of the review, which is an important factor as the publication time-lag outdates the results of the reviews in some areas of investigation.

All articles retrieved from the initial electronic database search are, then, extracted to an Excel file (Microsoft® Office) and the duplicates are removed by software filter and verified manually. After this process, all titles, abstracts, and keywords of the obtained papers are screened. The identified relevant studies are retrieved and the respective full-text is analyzed for eligibility. The definition of the eligibility criteria depends on the purpose of the review and the information intended to analyze. However, some eligibility criteria are common to all topics approached in sections 2.2., 2.3 and 2.4. Conference proceedings, reviews and meta-analyses, case studies and/or expert opinions, and studies that are not written in the English language are not eligible and, therefore, are excluded.

After all the full-texts of the articles have been assessed for eligibility, the final set of articles to be included in the review is obtained. In this work, the list of references of the relevant articles that result from database search are carefully examined and analyzed in order to identify additional records to be included in the literature review. Customized data extraction tables are developed to extract key details from each included study. The extracted information depends on the topic of the review, and it is chosen to provide, for instance, an overview of the methods each study considers in the analyzes performed and of the results and conclusions obtained. When only partial information is described in the original article, the references and the authors' previous works are analyzed to provide comparable data across the selected studies.

The general flowchart of the research methodology adopted in this work to identify and select the studies to be included in literature reviews is presented in Figure 2.1.

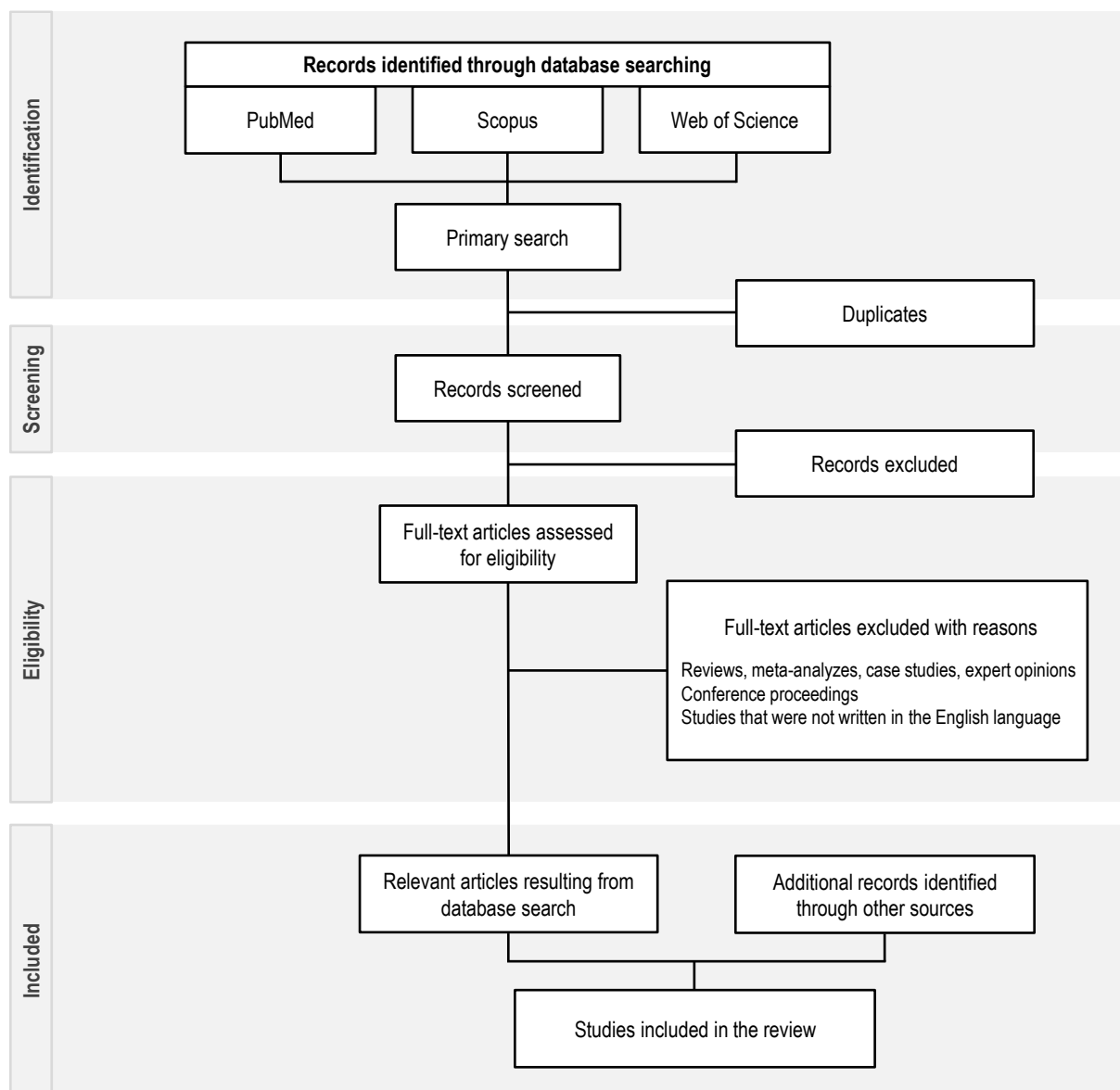


Figure 2.1 – Flowchart of the search strategy adopted to identify and select the papers to include in literature reviews.

2.2. Biomechanical Models for Device-Assisted Locomotion Analysis

A detailed evaluation of the characteristics utilized on currently existing biomechanical models of the human body analyzing locomotion aided by four specific types of mobility assistive devices, namely crutches, walkers, wheelchairs, and canes, is provided in this section. The methodology described in section 2.1. was applied on July 31, 2021. The established search strategy is the one presented in section 2.1 and an example for the PubMed database is depicted in Table 2.1.

Table 2.1 – Example of the search strategy for the PubMed database utilized to find biomechanical models for the analysis of device-assisted locomotion

Search number	Terms utilized	Results
#1	biomechanical [Title/Abstract]	55,221
#2	skeletal [Title/Abstract]	210,370
#3	musculoskeletal [Title/Abstract]	59,795
#4	musculo-skeletal [Title/Abstract]	1,394
#5	neuromusculoskeletal [Title/Abstract]	656
#6	#1 OR #2 OR #3 OR #4 OR #5 [Title/Abstract]	318,511
#7	model* [Title/Abstract]	3,188,805
#8	crutch* [Title/Abstract]	1,886
#9	cane* [Title/Abstract]	7,248
#10	walker* [Title/Abstract]	14,028
#11	wheelchair* [Title/Abstract]	7,918
#12	"assistive device" [Title/Abstract]	966
#13	"assistive devices" [Title/Abstract]	2,134
#14	"mobility aid" [Title/Abstract]	162
#15	"mobility aids" [Title/Abstract]	278
#16	"assisted walking" [Title/Abstract]	189
#17	#8 OR #9 OR #10 OR #11 OR #12 OR #13 OR #14 OR #15 OR #16 [Title/Abstract]	32,940
#18	#6 AND #7 AND #17 [Title/Abstract]	252

Apart from the standard exclusion criteria defined in section 2.1, some additional ones were considered. Studies were excluded if (i) they did not utilize biomechanical, skeletal, musculoskeletal or neuromusculoskeletal models; (ii) they did not utilize assistive devices; (iii) they utilized assistive devices not targeted in this work; (iv) they included finite element analysis; (v) they did not analyze assistive device-biomechanical model interaction; (vi) they analyzed sports activities; (vii) they analyzed patient handling; (viii) the assistive device use was temporary; (ix) they did not analyze device-assisted locomotion; and (x) they analyzed fatigue. Concerning exclusion criterion (vii), the analysis was carried out between the caregiver and the assistive device, and not between the device and the patient using it. Also, in the exclusion criterion (viii), the assistive device was not utilized as a habitual means of locomotion.

Database search provided a total of 1537 studies. After duplicate removal, 953 articles were screened, and 465 full texts were retrieved to be examined in detail. A total of 53 articles retrieved from database search met the eligibility criteria and were included in this work. After careful examination of the reference lists of those 53 studies, 19 additional ones were identified. Therefore, a total of 72 studies, dated from 1985 to 2021, were included and subjected to analysis. Amongst the included studies, 18, 10, 42, and 2 referred to the use of crutches, walkers, wheelchairs, and canes, respectively. A flowchart of the methodology conducted to obtain the results of this section is provided in Figure 2.2.

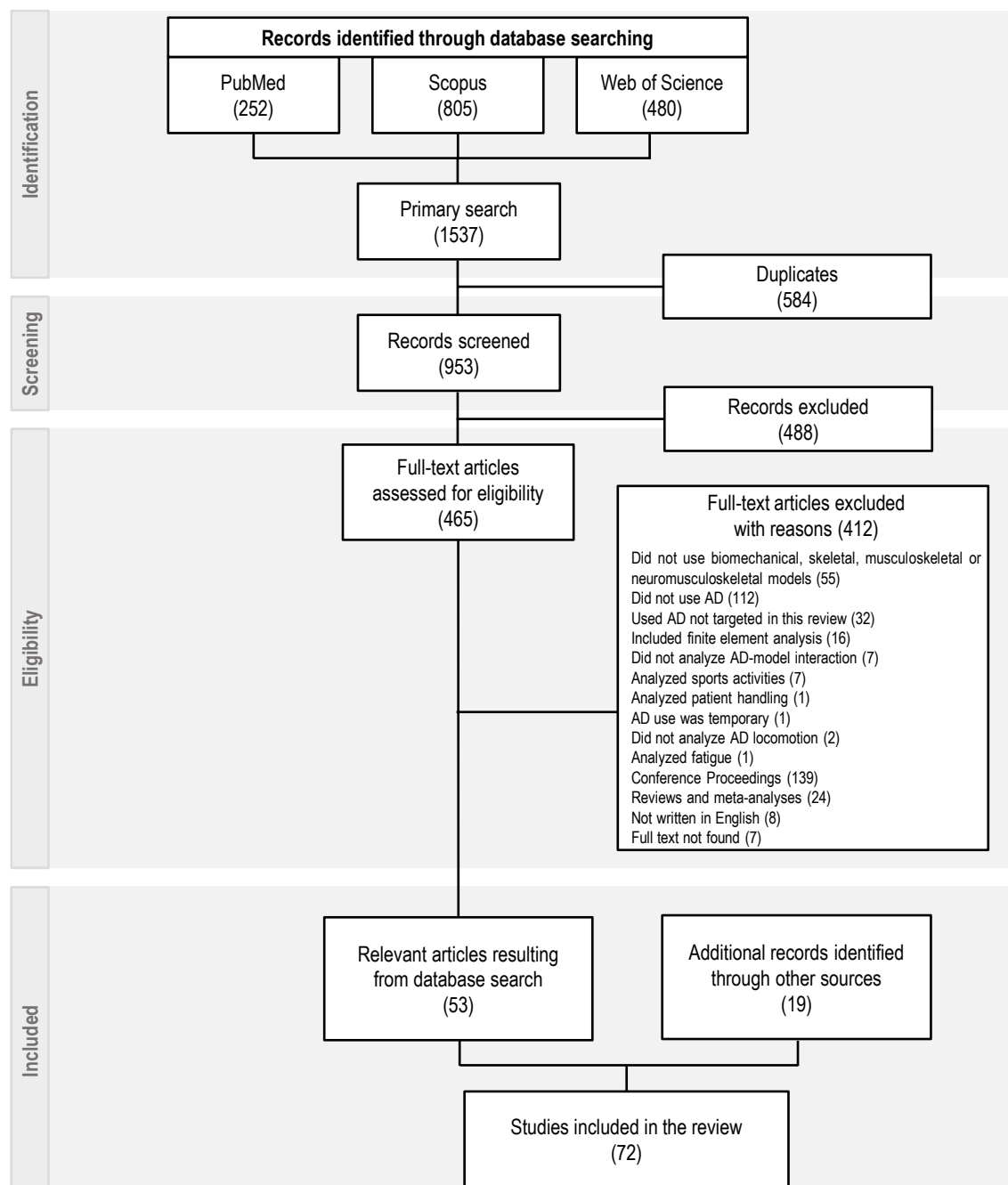


Figure 2.2 – Flowchart of the search methodology conducted in this section to find studies analyzing biomechanical modeling of device-assisted locomotion.

It is important to note that, during the analysis of the studies included in this section, a heterogeneity in reporting the joints of the shoulder joint complex was noted, as the term “shoulder” was utilized in some situations, not clearly specifying which of the articulations was considered, either the glenohumeral, the sternoclavicular, the acromioclavicular or the scapulothoracic joints. In order to provide a similar comparison basis across all studies, a homogenization of this terminology was carried out. When the study referred the term “shoulder” as the articulation of the shoulder joint complex of the biomechanical model, an investigation was carried out in order to determine which articulation was, in fact, considered. In this sense, the term “shoulder” is mentioned, followed by the articulation that is, in fact, considered in between parenthesis. Example: shoulder (glenohumeral).

Figure 2.3 depicts the time evolution of the studies analyzing device-assisted locomotion over the years. It can be observed that there was a clear growing tendency to expand the knowledge on this scientific area of investigation from 1985 to 2014, but from 2015 onwards a decreasing tendency is verified. However, contrary to this tendency, it is important to mention that the study of crutch-assisted locomotion has been rising since 1985, with all studies found in the period [2020-2021] being associated with this mobility assistive device. In general, wheelchairs were the most commonly studied device, and this can be concluded from the fact that the number of studies was the highest, representing more than half of the total number of studies found. The peak of study of wheelchair-assisted locomotion analysis was in the period [2010-2014], with the last studies being published in 2019. In addition, observing Figure 2.3, it can be concluded that walkers and canes have not been as much studied as the other two mobility assistive devices. In fact, canes were only explored by two studies in 1993 and 2000, which means that recent studies on the analysis of cane-assisted locomotion are not available.

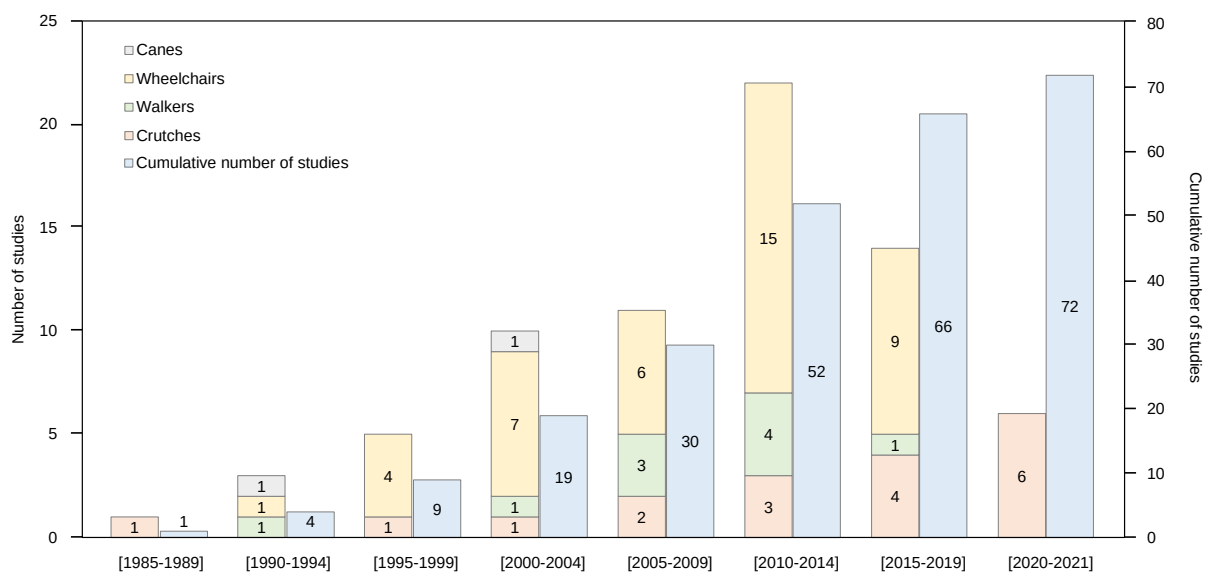


Figure 2.3 – Evolution of the number of studies analyzing device-assisted locomotion over the years.

The information extracted from the studies analyzing device-assisted locomotion is presented in Table 2.2. The information includes the characteristics of the biomechanical models utilized or developed by the studies, specifically the segments and joints, and it is organized in a chronological order and by assistive device, beginning with crutches, walkers, wheelchairs, and canes.

Table 2.2 – Characteristics of the biomechanical models of studies analyzing device-assisted locomotion

Author, Year	Characteristics of the Biomechanical Model
	Crutches
Reisman et al. (1985)	Dimension: 3D
Noreau et al. (1995)	Dimension: 2D Segments: thighs, legs, feet; head, trunk; arms; forearms, crutches Joints: shoulder (glenohumeral), elbow, hip
van der Spek et al. (2003)	Original model: van der Spek et al. (1998) Dimension: 2D Segments: thighs, legs, feet; head, arms, trunk (HAT) Joints: ankle, hip
Requejo et al. (2005)	Dimension: 3D Segments: thorax; right arm; left arm; right forearm; left forearm; right hand; left hand; right upper crutch; left upper crutch; right lower crutch; left lower crutch Joints: right glenohumeral; left glenohumeral; right elbow; left elbow; right wrist; left wrist
Slavens et al. (2009)	Dimension: 3D Segments: thorax; right arm; left arm; right forearm; left forearm; right hand; left hand; right crutch; left crutch Joints: right glenohumeral; left glenohumeral; right elbow; left elbow; right wrist; left wrist
Slavens et al. (2010)	Original models: Nguyen & Baker (2004), Requejo et al. (2005), Wu et al. (2005), Hingtgen et al. (2006) Dimension: 3D Segments: thorax; right arm; left arm; right forearm; left forearm; right hand; left hand; right crutch; left crutch Joints: right glenohumeral; left glenohumeral; right elbow; left elbow; right wrist; left wrist,
Carpentier et al. (2010)	Dimension: 2D Segments: legs; trunk; arms; forearms, crutches Joints: hip; shoulder (glenohumeral); elbow
Slavens, Bhagchandani, et al. (2011)	Original models: Poppen & Walker (1976), Veeger et al. (1997), Schmidt et al. (1999), Rab et al. (2002), Roux et al. (2002), Nguyen & Baker (2004), Wu et al. (2005), Slavens et al. (2010) Dimension: 3D Segments: thorax; right arm; left arm; right forearm; left forearm; right hand; left hand; right crutch handle; left crutch handle; right lower crutch; left lower crutch; right crutch cuff; left crutch cuff Joints: right glenohumeral; left glenohumeral; right elbow; left elbow; right wrist; left wrist
Lancini et al. (2016)	Dimension: 3D Segments: head, neck; thorax, abdomen; pelvis; right thigh; left thigh; right leg; left leg; right foot; left foot; right arm; left arm; right forearm, crutch; left forearm, crutch Joints: spine; neck; right shoulder (glenohumeral); left shoulder (glenohumeral); right elbow; left elbow; right hip; left hip; right knee; left knee; right ankle; left ankle

Perez-Rizo et al. (2017)	Original model: Requejo et al. (2005), Slavens, Bhagchandani, et al. (2011) Dimension: 3D Segments: thorax; arm; forearm; hand; crutch tip; crutch handle; crutch upper handlebar; crutch cuff Joints: shoulder (glenohumeral), elbow, wrist
Mouzo et al. (2018)	Dimension: 3D Segments: head; neck; thorax, abdomen; pelvis; right thigh; left thigh; right leg; left leg; right hindfoot; left hindfoot; right forefoot; left forefoot; right arm; left arm; right forearm; left forearm; right hand; left hand; right crutch; left crutch
Fournier et al. (2018)	Original model: AMS GaitFullBody model Dimension: 3D Segments: 37
Smith et al. (2020)	Original model: Fournier et al. (2018) Dimension: 3D
Pasinetti et al. (2020)	Original model: Lancini et al. (2016) Dimension: 3D Segments: head; thorax and abdomen; pelvis; right thigh; left thigh; right leg; left leg; right foot; left foot; right arm; left arm; right forearm, crutch; left forearm, crutch Joints: neck; back; right hip; left hip; right knee; left knee; right ankle; left ankle; right shoulder (glenohumeral); left shoulder (glenohumeral); right elbow; left elbow
Michaud et al. (2020)	Original model: Lúgrís, Carlin, Pàmies-Vilà, et al. (2013) Dimension: 3D Segments: head; neck; thorax, abdomen; pelvis; right thigh; left thigh; right leg; left leg; right hindfoot; left hindfoot; right forefoot; left forefoot; right arm; left arm; right forearm; left forearm; right hand; left hand; right crutch; left crutch
Payo et al. (2020)	Dimension: 3D Segments: arm; forearm; crutch Joints: shoulder (glenohumeral); elbow; wrist
Febrer-Nafria et al. (2020)	Original model: Hamner et al. (2010) Dimension: 3D Segments: head, neck, thorax, abdomen; pelvis; right thigh; left thigh; right leg; left leg; left foot; right foot; right arm; left arm; right forearm, hand; left forearm, hand; right crutch; left crutch Joints: lumbosacral; right shoulder (glenohumeral); left shoulder (glenohumeral); right elbow; left elbow; right hip; left hip; right knee; left knee; right ankle; left ankle
Febrer-Nafria et al. (2021)	Original model: Rajagopal et al. (2016) Dimension: 3D Joints: lumbo-sacral; right shoulder (glenohumeral); left shoulder (glenohumeral); right elbow; left elbow; right wrist; left wrist; right hip; left hip; right knee; left knee; right ankle; left ankle; right metatarsal; left metatarsal
Walkers	
Crosbie (1993)	Dimension: 2D Segments: trunk; arm; forearm; thigh; leg; foot; walker Joints: shoulder (glenohumeral); elbow; hip; knee; ankle
Bachschmidt et al. (2001)	Dimension: 3D Segments: trunk; right arm; left arm; right forearm; left forearm; right hand; left hand Joints: glenohumeral; elbow; wrist
Ming et al. (2008)	Dimension: 3D Segments: trunk; right arm; left arm; right forearm; left forearm Joints: glenohumeral; elbow

Ming et al. (2009)	Original model: Requejo et al. (2005) Dimension: 3D Segments: thorax; right arm; left arm; right forearm; left forearm; right hand; left hand Joints: right glenohumeral; left glenohumeral; right elbow; left elbow; right wrist; left wrist
Konop et al. (2009)	Dimension: 3D Segments: trunk; arm; forearm; hand Joints: glenohumeral; elbow; wrist
Takanokura (2010)	Dimension: 2D Segments: trunk, head; arm; forearm, hand Joints: chest; shoulder (glenohumeral); elbow
Audu et al. (2011)	Original models: Delp et al. (1990), Zhao et al. (1998) Dimension: 3D Segments: 21 Joints: 21, including toe-foot, ankle and subtalar, knee, patella-tibia, hip, six joints at the lumbar region, thorax-arm joint (glenohumeral)
Konop et al. (2011)	Original model: Bachschmidt et al. (2001), Baker et al. (2003), Strifling et al. (2008), Konop et al. (2009) Dimension: 3D Joints: glenohumeral; elbow; wrist
Nekoukar & Erfanian (2013)	Dimension: 2D Segments: trunk, head, pelvis; right thigh; left thigh; right leg; left leg; right foot; left foot; right arm; left arm; right forearm; left forearm; walker Joints: right hip; left hip; right knee; left knee; right ankle; left ankle; right shoulder (glenohumeral); left shoulder (glenohumeral); right elbow; left elbow; right wrist; left wrist
Taghvaei et al. (2017)	Dimension: 2D Segments: trunk, head; thigh; leg Joints: hip; knee; ankle
Wheelchairs	
Veeger et al. (1991)	Dimension: 3D Segments: arm; forearm; hand Joints: glenohumeral; elbow; wrist
Rao et al. (1996)	Dimension: 3D Segments: thorax; arm; forearm; hand Joints: glenohumeral; elbow; wrist
Rodgers et al. (1998)	Dimension: 3D Segments: arm; forearm; hand Joints: shoulder (glenohumeral); elbow; wrist
Kulig et al. (1998)	Dimension: 3D Segments: thorax; arm; forearm; hand Joints: shoulder (glenohumeral); elbow; wrist
Cooper et al. (1999)	Original model: Hanavan (1966) Dimension: 3D Segments: head; trunk; arm; forearm; hand Joints: neck; glenohumeral; elbow; wrist
Kulig et al. (2001)	Original model: Kulig et al. (1998) Dimension: 3D
Richter (2001)	Dimension: 2D Segments: arm; forearm, hand; handrim; wheel Joints: shoulder (glenohumeral); elbow

Koontz et al. (2002)	Original model: Cooper et al. (1999) Dimension: 3D Segments: trunk; arm; forearm; hand Joints: glenohumeral; elbow; wrist
Morrow et al. (2003)	Dimension: 2D Segments: arm; forearm; hand-wheel axle; shoulder (glenohumeral)-wheel axle Joints: shoulder (glenohumeral); elbow
Guo, Su, et al. (2003)	Dimension: 3D Segments: arm; forearm; hand Joints: shoulder (glenohumeral); elbow; wrist
Guo, Zhao, et al. (2003)	Dimension: 2D Segments: arm; forearm; hand-wheel axle; shoulder (glenohumeral)-wheel axle Joints: shoulder (glenohumeral); elbow
Lin et al. (2004)	Original model: Lin et al. (2001) Dimension: 3D Segments: trunk; arm; forearm; hand Joints: glenohumeral; elbow; wrist
Mercer et al. (2006)	Original model: Cooper et al. (1999) Dimension: 3D Segments: trunk; arm; forearm; hand Joints: glenohumeral; elbow; wrist
Desroches et al. (2008)	Original model: Dumas et al. (2004) Dimension: 3D Joints: shoulder (glenohumeral)
Collinger et al. (2008)	Original model: Cooper et al. (1999) Dimension: 3D
Dubowsky et al. (2008)	Dimension: 3D Segments: skull; spine; thorax, abdomen; pelvis; right scapula; left scapula; right clavicle; left clavicle; right humerus; left humerus; right radius; left radius; right ulna; left ulna; right hand; left hand
Sasaki et al. (2008)	Dimension: 3D Joints: shoulder (glenohumeral); elbow; wrist
Lombardi & Dedini (2009)	Dimension: 2D Segments: arm; forearm; hand Joints: shoulder (glenohumeral); elbow; wrist
Morrow, Hurd, et al. (2010)	Dimension: 3D Segments: thorax, abdomen; right arm; right forearm; right hand Joints: shoulder (glenohumeral); elbow; wrist
Gil-Agudo, Del Ama-Espinosa, Pérez-Rizo, Pérez-Nombela, & Crespo-Ruiz (2010)	Dimension: 3D Segments: thorax; forearm; arm; hand Joints: shoulder (glenohumeral); elbow; wrist
Morrow, Kaufman, et al. (2010)	Original model: Morrow, Hurd, et al. (2010) Dimension: 3D Segments: thorax, abdomen; arm; forearm; hand Joints: shoulder (glenohumeral); elbow; wrist
Rankin et al. (2010)	Original model: Holzbaur et al. (2005) Dimension: 3D Segments: thorax; right arm; right forearm; right hand Joints: shoulder (glenohumeral); elbow; forearm pronation and supination

Gil-Agudo, Del Ama-Espinosa, Pérez-Rizo, Pérez-Nombela, & Crespo-Ruiz (2010)	Original model: Gil-Agudo, Del Ama-Espinosa, Pérez-Rizo, Pérez-Nombela, & Crespo-Ruiz (2010) Dimension: 3D
Lin et al. (2011)	Dimension: 2D Segments: arm; forearm; hand-wheel axle; shoulder (glenohumeral)-wheel axle Joints: shoulder (glenohumeral); elbow; wrist
Rankin et al. (2011)	Original model: Holzbaur et al. (2005), Rankin et al. (2010) Dimension: 3D Segments: thorax; right arm; right forearm; right hand Joints: shoulder (glenohumeral); elbow; wrist
Munaretto et al. (2012)	Original model: Richter (2001), Guo, Zhao, et al. (2003) Dimension: 2D Segments: arm; forearm Joints: shoulder (glenohumeral); elbow; wrist
Rankin et al. (2012)	Original models: Holzbaur et al. (2005), Rankin & Neptune (2010), Rankin et al. (2011) Dimension: 3D Segments: thorax; right arm; right forearm; right hand Joints: shoulder (glenohumeral); elbow; wrist
Leary et al. (2012)	Original model: Richter (2001) Dimension: 2D
Slowik & Neptune (2013)	Original models: Holzbaur et al. (2005), Rankin et al. (2010), Rankin et al. (2011) Dimension: 3D Segments: thorax; right arm; right forearm; right hand Joints: shoulder (glenohumeral); elbow; wrist
Munaretto et al. (2013)	Original model: Munaretto et al. (2012) Dimension: 2D Segments: arm; forearm Joints: shoulder (glenohumeral); elbow; wrist
Schnorenberg et al. (2014)	Original models: Konop et al. (2009), Slavens et al. (2009), Slavens et al. (2010), Slavens, Graf, et al. (2011), Slavens, Bhagchandani, et al. (2011) Dimension: 3D Segments: thorax; right clavicle; left clavicle; right scapula; left scapula; right arm; left arm; right forearm; left forearm; right hand; left hand Joints: right glenohumeral; left glenohumeral; right acromioclavicular; left acromioclavicular right sternoclavicular; left sternoclavicular; right elbow; left elbow; right wrist; left wrist
Morrow et al. (2014)	Original models: Holzbaur et al. (2005), Rankin et al. (2011) Dimension: 3D Segments: thorax; right arm; right ulna; right radius; right hand Joints: shoulder (glenohumeral); elbow
Gil-Agudo et al. (2014)	Original model: Gil-Agudo, del Ama-Espinosa, Pérez-Rizo, Pérez-Nombela, & Crespo-Ruiz (2010) Dimension: 3D
Slavens, Schnorenberg, Aurit, Graf, et al. (2015)	Original model: Schnorenberg et al. (2014) Dimension: 3D Segments: thorax; right clavicle; left clavicle; right scapula; left scapula; right arm; left arm; right forearm; left forearm; right hand; left hand Joints: right glenohumeral; left glenohumeral; right acromioclavicular; left acromioclavicular right sternoclavicular; left sternoclavicular; right elbow; left elbow; right wrist; left wrist

Slavens, Schnorenberg, Aurit, Tarima, et al. (2015)	Original model: Schnorenberg et al. (2014) Dimension: 3D Segments: thorax; right clavicle; left clavicle; right scapula; left scapula; right arm; left arm; right forearm; left forearm; right hand; left hand Joints: right glenohumeral; left glenohumeral; right acromioclavicular; left acromioclavicular; right sternoclavicular; left sternoclavicular; right elbow; left elbow; right wrist; left wrist
Slowik et al. (2016)	Original models: Holzbaur et al. (2005), Rankin et al. (2010), Rankin et al. (2011) Dimension: 3D Segments: thorax; right arm; right forearm; right hand Joints: shoulder (glenohumeral); elbow; wrist
Hernandez et al. (2018)	Original models: Delp et al. (1990), Holzbaur et al. (2005) Dimension: 3D Segments: trunk; arm; forearm; hand Joints: pelvic girdle joint; shoulder (glenohumeral); elbow; wrist
Hybois et al. (2018)	Original model: Saul et al. (2015) Dimension: 3D Segments: thorax; clavicle; scapula; humerus; ulna; radius; hand
Kurup et al. (2019)	Original model: Saul et al. (2015) Dimension: 3D Segments: thorax; right arm; right ulna; right radius; right hand Joints: shoulder (glenohumeral); elbow; wrist
Odle et al. (2019)	Original model: OpenSim Arm 23 model Dimension: 3D Segments: spine; rib cage; clavicle; scapula; humerus; ulna; radius; hand Joints: shoulder (glenohumeral); elbow; forearm pronation and supination; wrist
Hybois et al. (2019)	Dimension: 3D Segments: thorax, clavicle, scapula, arm, forearm, hand Joints: glenohumeral, elbow, wrist
Puchaud et al. (2019)	Original model: Vasavada et al. (1998), Holzbaur et al. (2005) Dimension: 3D Segments: head; thorax; right clavicle; left clavicle; right scapula; left scapula; right humerus; left humerus Joints: right glenohumeral; left glenohumeral; right acromioclavicular; left acromioclavicular; right scapulothoracic; left scapulothoracic; right sternoclavicular; left sternoclavicular
Canes	
Winter et al. (1993)	Dimension: 2D Segments: hand, cane; forearm; arm Joints: shoulder (glenohumeral); elbow; wrist
Anglin et al. (2000)	Original models: Karlsson & Peterson (1992), (Veeger et al., 1997) Dimension: 3D Segments: thorax; humerus; scapula; clavicle; ulna; radius Joints: glenohumeral; sternoclavicular; acromioclavicular; scapulothoracic

The studies considered a variety of characteristics for the biomechanical model. Observing Table 2.2, the majority of the studies utilized spatial or three-dimensional (3D) models (78%), while planar or two-dimensional (2D) models were used in 22% of the studies. The topology is an important characteristic of the biomechanical models and different levels of complexity were found and are reported in Table 2.2. The studies utilized either full-body models or models representing the upper extremities only. Concerning

upper extremity models, these can further be classified as bilateral or unilateral, depending on whether they include both the right and left sides of the human body or include one side only, respectively. More than half of the studies considered upper extremity models. Some studies did not provide information on this topic. Figure 2.4 presents the distribution of the topology of the biomechanical models.

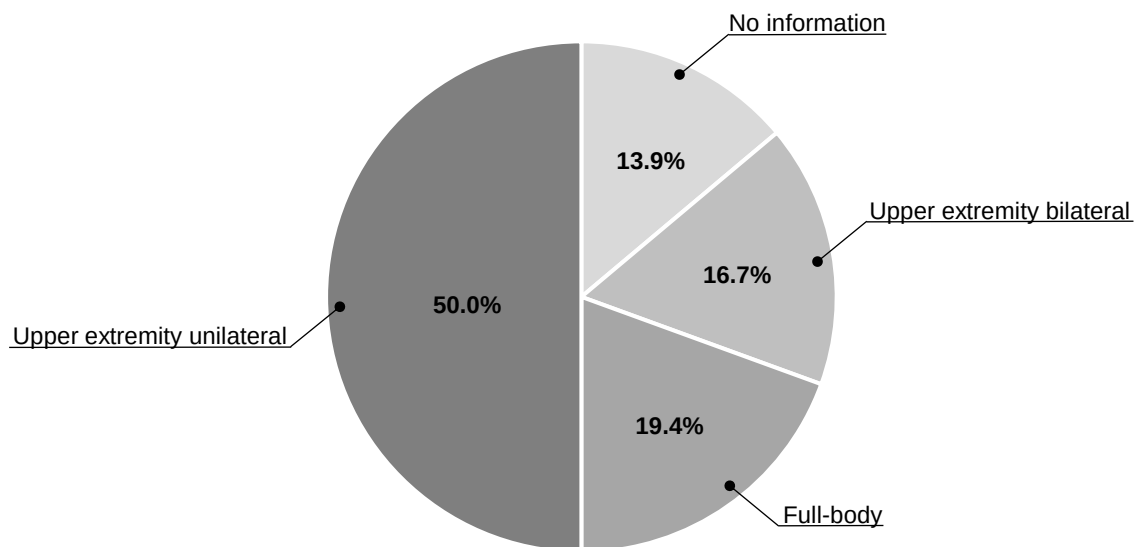


Figure 2.4 – Distribution of the topology of the biomechanical models of the studies included in this section.

As stated in section 1.1., device-assisted locomotion places substantial and repetitive demands on the upper extremities, which are not adapted to weight-bearing tasks. These loads are transmitted to the hand, wrist, forearm, elbow, arm and shoulder and must be accurately captured by the biomechanical models. In general, biomechanical studies typically concentrate on the analysis of the lower extremity, while the upper extremity receives less attention. Among the studies displayed in Table 2.2, only 58 reported the joints of the biomechanical models. The majority of those 58 studies represented the shoulder joint by means of the glenohumeral joint only, connecting the thorax and the arm/humerus segments. On the other hand, among all the studies, only five utilized a detailed model for the shoulder joint, including the glenohumeral, acromioclavicular, sternoclavicular and scapulothoracic joints. A more detailed model for the shoulder implies the use of two additional segments besides the thorax and the arm/humerus, specifically the clavicle and the scapula. This modeling approach provides a more realistic representation of the movements allowed by the shoulder joint complex, which might be beneficial for studying device-assisted locomotion. It is important to note that those five studies analyzed wheelchair- and cane-assisted locomotion. Some studies considered the forearm as one unique segment, while others modeled the radius and the ulna independently. Elbow flexion and extension was considered in the majority of studies, but few have taken into consideration the forearm pronation and supination. The radial and ulnar deviation was not considered.

2.3. Crutch Modeling Procedures

As concluded in section 2.2, the research and interest in studying crutch-assisted locomotion has been rising over the last years. This rising tendency is evident from the fact that more than half of the studies on crutch locomotion were published after 2010 (see Figure 2.3). Thus, the present section provides a detailed analysis of currently existing biomechanical modeling approaches that investigate this topic. One of the most critical and challenging aspects when studying crutch locomotion is the interfaces between the crutch and the surrounding environment, namely the ground and human body. Crutch-body interface develops at the hand, and forearm or axilla, depending on the type of crutch utilized (see Figure 1.1c). The modeling process of the interfaces is complex as it is strongly dependent on multiple factors, including the geometry and local physical properties of the contacting surfaces, thus influencing the dynamic response of the biomechanical model. Appropriate modeling and numerical descriptions of these interfaces are required to accurately replicate the human movement during crutch-assisted locomotion.

Crutches allow a wide range of gait patterns, namely two-point, three-point, or four-point reciprocal gait, and swing-through and swing-to gait patterns. The type of crutch-assisted gait pattern is prescribed by therapists and depends on the injury and condition of the patient (Lindh et al., 2009). Table 2.3 provides a comparison amongst the different types of crutch-assisted gait patterns, and Figure 2.5 illustrates the differences between them.

Table 2.3 – Types of crutch-assisted gait patterns and their characteristics (Lindh et al., 2009; Subhash, 2011)

Gait pattern		Characteristics
Reciprocal gait	Two-point	Utilized when the patients' balance is good Some amount of body weight can be borne by both limbs, which are weak Gait sequence (example): left crutch and right foot; right crutch and left foot
	Three-point	Utilized by patients who can only bear partial weight on one leg or just touch the ground with the foot of that leg Both crutches and the weak leg move at the same time Gait sequence (example): both crutches and right foot; left foot
	Four-point	Utilized by patients who are able to bear weight on both legs and can move each leg separately Slower gait pattern Gait sequence (example): right crutch; left foot; left crutch; right foot
Swing-through gait		Utilized when the patient is not capable of moving the lower limbs individually due to paralysis The feet are placed slightly in front of the crutches Gait sequence (example): both crutches; both feet
Swing-to gait		Utilized when the patient is not capable of moving the lower limbs individually due to paralysis The feet are placed in the same location as the crutches Gait sequence (example): both crutches; both feet

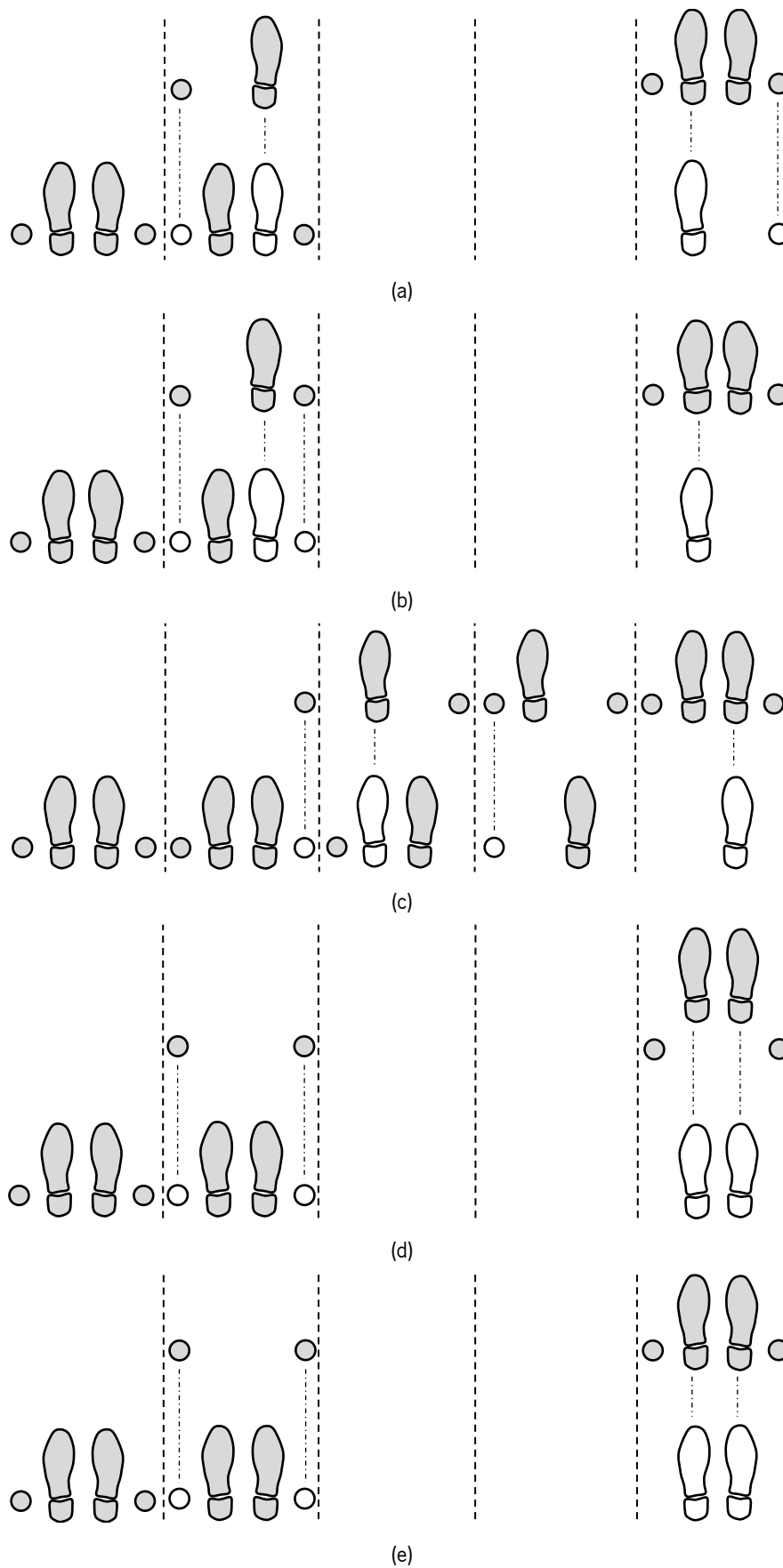


Figure 2.5 – Types of crutch-assisted gait patterns. (a) Two-point reciprocal gait. (b) Three-point reciprocal gait. (c) Four-point reciprocal gait. (d) Swing-through gait. (e) Swing-to gait.

The methodology described in section 2.1. was applied for this topic of investigation on November 6, 2023, with no restrictions on the year of publication. The search strategy was defined using the Boolean operators AND/OR and was established combining a carefully selected list of keywords as

SET 1: skeletal OR musculoskeletal OR musculo-skeletal OR neuromusculoskeletal OR biomechanic* OR multibody

SET 2: model* OR system

SET 3: crutch*

Search strategy: SET 1 AND SET 2 AND SET 3

An example of the search strategy for the PubMed database is presented in Table 2.4.

Table 2.4 – Example of the search strategy for the PubMed database utilized to find biomechanical models for crutch-assisted locomotion analysis

Search number	Terms utilized	Results
#1	skeletal [Title/Abstract]	233,870
#2	musculoskeletal [Title/Abstract]	73,236
#3	musculo-skeletal [Title/Abstract]	1,479
#4	neuromusculoskeletal [Title/Abstract]	846
#5	biomechanic* [Title/Abstract]	88,315
#6	multibody [Title/Abstract]	1,091
#7	#1 OR #2 OR #3 OR #4 OR #5 OR #6 [Title/Abstract]	386,361
#8	model* [Title/Abstract]	3,860,267
#9	system [Title/Abstract]	2,794,480
#10	#8 OR #9 [Title/Abstract]	6,113,942
#11	crutch* [Title/Abstract]	2,072
#12	#7 AND #10 AND #11 [Title/Abstract]	65

Besides the standard exclusion criteria defined in section 2.1, in this section, studies were excluded based on the following criteria: (i) the study did not use biomechanical, skeletal, musculoskeletal or neuromusculoskeletal models; (ii) the study did not consider the use of crutches.

The initial database search provided a total of 465 studies, 65 from PubMed, 315 from Scopus and 85 from Web of Science. After removing the duplicated studies, 335 articles were screened, and 124 full texts were retrieved to be examined in detail. A total of 23 articles retrieved from database search, dated from 1985 to 2023, met the eligibility criteria and were included in this work. After careful examination of the references lists of those 23 studies, an additional study was identified, included, and subjected to analysis. The flowchart of the research methodology conducted in this section is provided in Figure 2.6.

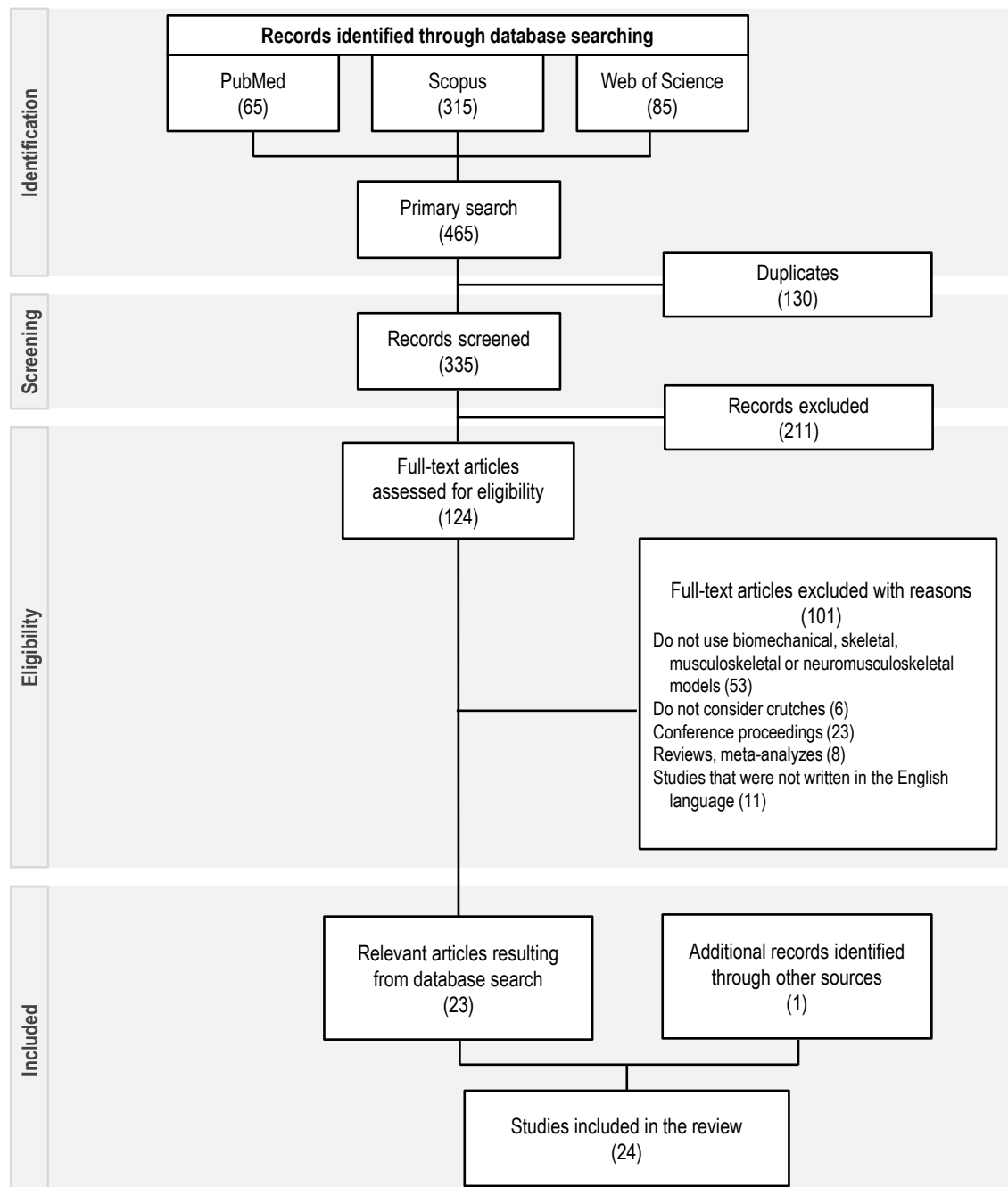


Figure 2.6 – Flowchart of the methodology conducted in this section to find studies analyzing crutch-assisted locomotion.

The full-text of the articles was analyzed and information on crutch-assisted gait modeling was extracted to a customized table (see Table 2.5), considering the following aspects: (i) type of considered crutch, (ii) analyzed movement, (iii) modeling approach employed to introduce the crutches in the model, (iv) crutch-model interface and (v) crutch-ground interface. This set of characteristics was selected in order to provide an overview of the methodology developed in each article and to allow a discussion of the obtained results and of the reached conclusions. Whenever the original paper provided partial information only, its references and the authors' previous publications were carefully analyzed. In Table 2.5, the information is organized in a chronological order.

Table 2.5 – Crutch modeling procedures employed in the studies included in this section

Author, Year	Crutch Modeling Procedure
Reisman et al. (1985)	Type: axillary Movement: swing-through gait Approach: crutches as massless elements Crutch-model interface: no information Crutch-ground interface: reaction forces on the crutch tip recorded with a force plate
Rovick & Childress (1988)	Type: forearm Movement: swing-through gait Approach: arms, forearms, and crutches as one rigid body Crutch-model interface: not applicable Crutch-ground interface: revolute joint between the crutch tip and the ground
Noreau et al. (1995)	Type: forearm Movement: swing-through gait Approach: forearms and crutches as one rigid body Crutch-model interface: not applicable Crutch-ground interface: reaction forces on the crutch tip recorded with a force plate
Tashman et al. (1995)	Type: forearm Movement: reciprocal gait Approach: upper extremities and crutches not explicitly included in the model Crutch-model interface: set of moments and forces acting on the shoulders Crutch-ground interface: reaction forces on the crutch tip recorded with a force plate
van der Spek et al. (2003)	Type: forearm Movement: standing Approach: upper extremities and crutches not explicitly included in the model and considered as massless elements Crutch-model interface: constraint force holding the tip of the crutch and the shoulder joint at a constant distance Crutch-ground interface: crutch-ground reaction force with equal magnitude and opposite direction as the constraint force
Requejo et al. (2005)	Type: forearm Movement: four-point reciprocal gait Approach: crutches as rigid bodies Crutch-model interface: crutches instrumented with six load cells and strain gauges to determine crutch forces and moments Crutch-ground interface: reaction forces on the crutch tip collected from a force plate and crutches instrumented with transducers
Slavens et al. (2009)	Type: forearm Movement: swing-through and reciprocal gait Approach: crutches as rigid bodies Crutch-model interface: no information Crutch-ground interface: reaction forces on the crutch tip collected from a force plate and crutches instrumented with transducers
Carpentier et al. (2010)	Type: forearm Movement: no information Approach: forearms and crutches as one rigid body Crutch-model interface: not applicable Crutch-ground interface: impulsive contact forces on the tip of the crutch

Slavens et al. (2010)	Type: forearm Movement: swing-through and reciprocal gait Approach: crutches as rigid bodies Crutch-model interface: the forces and moments at the crutch-hand interface calculated from the transducer output Crutch-ground interface: reaction forces and moments on the crutch tip collected from a force plate and crutches instrumented with transducers
G. Liu et al. (2011)	Type: spring-loaded axillary Movement: swing-through gait Approach: crutches not explicitly included in the model and considered massless and elastic Crutch-model interface: constraint force along the crutch axis applied to the model Crutch-ground interface: revolute joint between the crutch tip and the ground
Slavens, Bhagchandani, et al. (2011)	Type: forearm Movement: two-point reciprocal gait Approach: crutches as rigid bodies Crutch-model interface: force transducers placed above the crutch handle to measure reaction forces and moments Crutch-ground interface: force transducers placed below the crutch handle to measure reaction forces and moments; reactions at the tip-ground interface calculated by the model and collected from force plate
Font-Llagunes et al. (2012)	Type: forearm Movement: swing-through gait Approach: forearms and crutches as one rigid body Crutch-model interface: not applicable Crutch-ground interface: single point of contact model between the crutch tip and the ground; impulsive bilateral constraints and compliant contact force models
Lugris, Carlin, Luaces, et al. (2013)	Type: forearm Movement: no information Approach: crutches as rigid bodies Crutch-model interface: crutches rigidly connected to the hands; reaction forces on the crutch cuff recorded with strain gauge-based load cells; cuff reactions as a normal force acting on its middle point Crutch-ground interface: reaction forces on the crutch tip recorded with strain gauges; ground reaction as a force acting at the tip center
Lancini et al. (2016)	Type: forearm Movement: no information Approach: forearms and crutches as one rigid body Crutch-model interface: not applicable Crutch-ground interface: reaction forces on the crutch tip recorded with strain gauges; ground reaction as external constraint at the tip
Perez-Rizo et al. (2017)	Type: forearm Movement: swing-through and two-point reciprocal gait Approach: crutches as rigid bodies Crutch-model interface: reaction forces on the crutch cuff recorded with strain gauges; crutch handle-hand forces applied at the projection of the center of the third metacarpal head on the longitudinal axis of the crutch handle; lateral/longitudinal crutch-forearm forces and moments in all directions considered negligible; anteroposterior crutch-forearm forces applied on the forearm Crutch-ground interface: reaction forces and moments on the crutch tip recorded with strain gauges

Fournier et al. (2018)	Type: forearm Movement: no information Approach: no information Crutch-model interface: normal crutch cuff-forearm forces applied using virtual muscles; crutch handle-hand forces applied in all directions Crutch-ground interface: reaction forces on the crutch tip recorded with strain gauges
Mouzo et al. (2018)	Type: forearm Movement: no information Approach: crutches as rigid bodies Crutch-model interface: crutches rigidly connected to the hands; reaction forces on the crutch cuff recorded with strain gauges Crutch-ground interface: reaction forces on the crutch tip recorded with strain gauges
Michaud et al. (2020)	Type: forearm Movement: four-point reciprocal gait Approach: crutches as rigid bodies Crutch-model interface: crutches rigidly connected to the hands; reaction forces on the crutch cuff recorded with strain gauges, but they were not utilized in the model as the hands and crutches are rigidly connected Crutch-ground interface: reaction forces on the crutch tip recorded with strain gauges
Febrer-Nafria et al. (2020)	Type: forearm Movement: four-point reciprocal gait Approach: crutches as rigid bodies Crutch-model interface: crutches rigidly connected to the forearms-hands Crutch-ground interface: reaction forces on crutch tip recorded with tri-axial load cells
Payo et al. (2020)	Type: forearm Movement: swing-through and two-point reciprocal gait Approach: crutch as a rigid body Crutch-model interface: reaction forces on the crutch cuff recorded with an axial force sensor; the moment at the crutch cuff is considered to be negligible Crutch-ground interface: reaction forces on the crutch tip recorded with a six-axis force sensor; the moment at the crutch cuff considered to be negligible
Pasinetti et al. (2020)	Type: forearm Movement: no information Approach: forearms and crutches as one rigid body; the influence of each crutch considered by adding 1.5 kg to each forearm Crutch-model interface: no information Crutch-ground interface: axial reaction forces recorded with strain gauges
Smith et al. (2020)	Type: forearm Movement: four-point reciprocal gait Approach: no information Crutch-model interface: normal reaction forces of the crutch cuff applied between the cuff and the forearm; reaction forces of the crutch handle and hand applied in all directions Crutch-ground interface: axial reaction force on the crutch tip recorded with strain gauges
Febrer-Nafria et al. (2021)	Type: forearm Movement: four-point reciprocal gait Approach: crutches as rigid bodies Crutch-model interface: crutches rigidly connected to the hands Crutch-ground interface: reaction forces on the crutch tip recorded with strain gauges; normal and tangential crutch-ground contact model considering a sphere at the crutch tip and a plane representing the ground

Ghidelli et al. (2023)	Type: forearm Movement: two-point and three-point reciprocal gait Approach: crutch as a rigid body Crutch-model interface: crutches rigidly connected to the hands Crutch-ground interface: reaction forces on the crutch tip recorded with strain gauges
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In what concerns to crutch modeling procedures, more than 90% of the included studies analyzed forearm crutches, and Reisman et al. (1985) and G. Liu et al. (2011) explored axillary crutch modeling. In addition, the studied movements comprised gait and standing. Standing was explored by one study only. Seven studies did not report this information. The considered gait patterns included swing-through and reciprocal gait (see Figure 2.5). Among the reciprocal gait, ten studies reported the type of pattern considered as two-point, three-point or four-point reciprocal gait. Three studies utilized reciprocal gait but did not provide further information. Five studies analyzed both swing-through and reciprocal gait patterns. Swing-to gait was not investigated. Three approaches were identified for incorporating the crutches into biomechanical models, namely considering (i) the crutch as a massless element not explicitly included in the model, (ii) the crutch and other body of the biomechanical model as a unique segment, and (iii) the crutch as an independent rigid body. The bodies with which the crutches were considered as a unique segment include the entire upper extremity and the forearms. Two studies did not state the considered crutch modeling approach. Figure 2.7 depicts the crutch modeling approaches identified in this section.

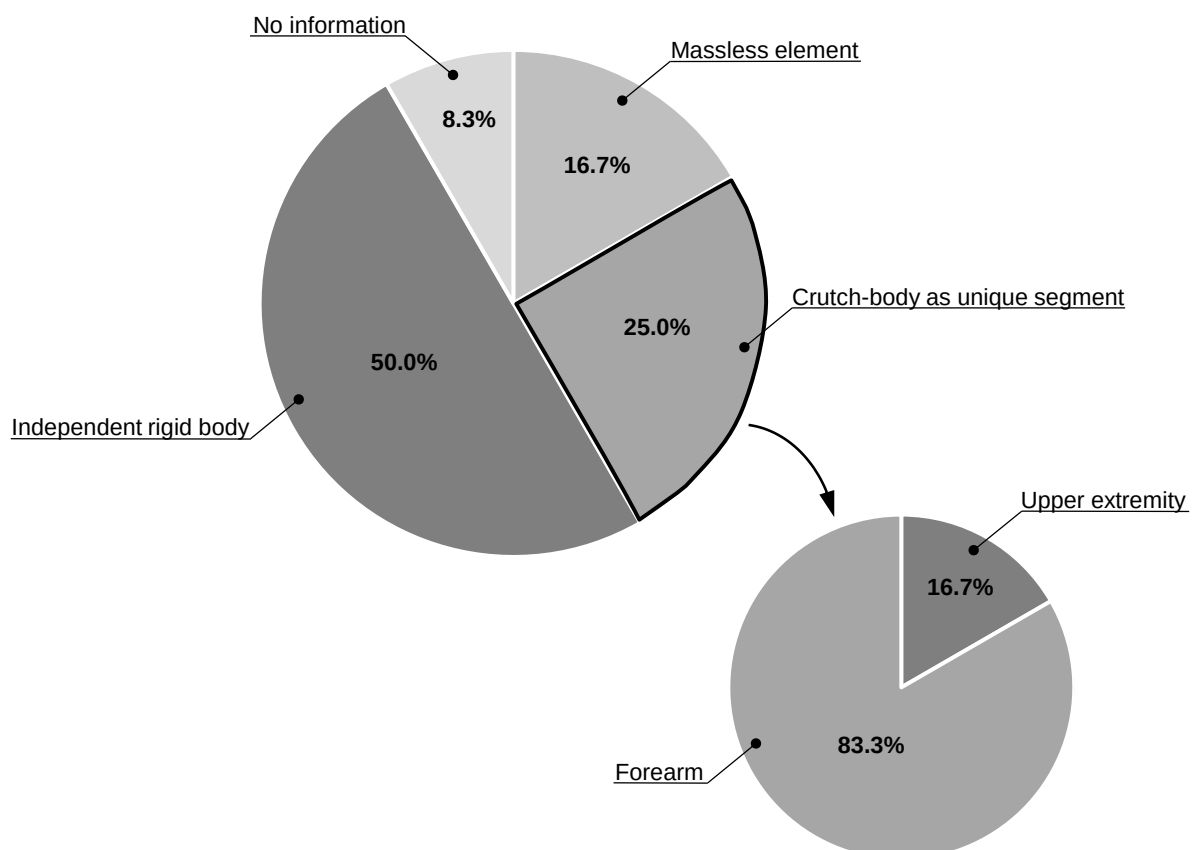


Figure 2.7 – Distribution of the crutch modeling approaches considered in the studies included in this section.

During unassisted gait, the only interaction with the environment occurs through the feet when there is contact with the ground (Cenk Güler et al., 1998; Millard & Mombaur, 2019; Morales-Orcajo et al., 2016; Saraiva et al., 2022; Shourijeh & McPhee, 2015; M. R. Silva et al., 2022b). However, during device-assisted locomotion, besides the foot-ground interaction, other sources of contact must be taken into consideration, specifically device-ground and device-model interactions. The accurate determination of the reaction forces and moments associated with these contacts is crucial as they influence the correct calculation of the joint reaction forces and moments directly related to the movement under analysis. In this situation, the data provided by the optical motion capture systems and force platforms are not sufficient to determine the joint reaction forces and moments, and other approaches must be considered.

A variety of strategies for modeling the interface that exists between the crutch and the biomechanical model was found. Some studies quantified the forces and moments at the cuff and/or handle with the use of crutches instrumented with sensors, while others considered the crutch rigidly connected to forearms or hands. Rigidly connecting the crutch to a body of the biomechanical model restrains the relative translation and rotation of the crutch with respect to that body and, thus, removes the associated six degrees-of-freedom. Other strategies employed virtual muscles and applied forces and/or moments to the utilized biomechanical model. Some studies did not provide information on the crutch-model interface. It is important to note that, in some cases, the same study applied more than one strategy for determining the interface between the crutch and the biomechanical model. For the studies that assumed the crutch and other body of the biomechanical model as a unique segment (see Figure 2.7), the crutch-model interface does not exist. Figure 2.8 displays the distribution of the approaches for crutch-model interface.

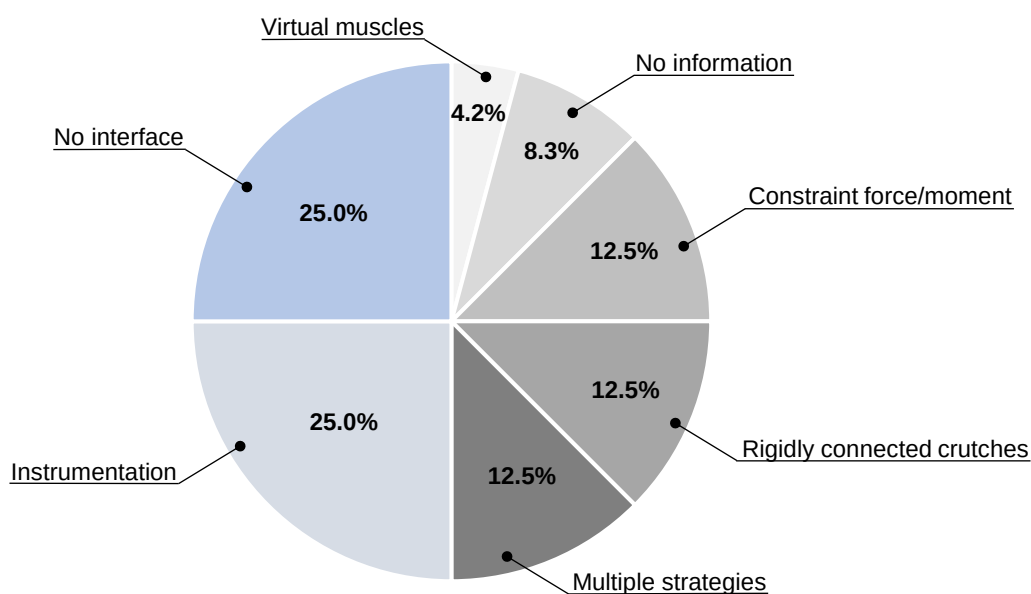


Figure 2.8 – Distribution of the approaches for crutch-model interface considered in the studies included in this section.

Five strategies for modeling the interface between the crutch and the ground were identified. The majority of the included studies utilized crutches instrumented with sensors to measure the forces and moments on the crutch tip or below the crutch handle, while others recorded the reaction forces of the crutch with the ground with force plates or considered a revolute joint between the crutch tip and the ground. The use of a revolute joint between the tip and the ground disregards their relative sliding motion. One study applied a constraint force holding the tip of the crutch and the shoulder joint at a constant distance, and, thus, the crutch-ground reaction force had equal magnitude and opposite direction as the constraint force. More recently, two studies considered contact models to address the crutch-ground interface. It is important to note that, in five cases, the same study applied more than one strategy for determining the interface between the crutch and the ground. Figure 2.9 shows the distribution of the approaches for crutch-ground interface found in the present section.

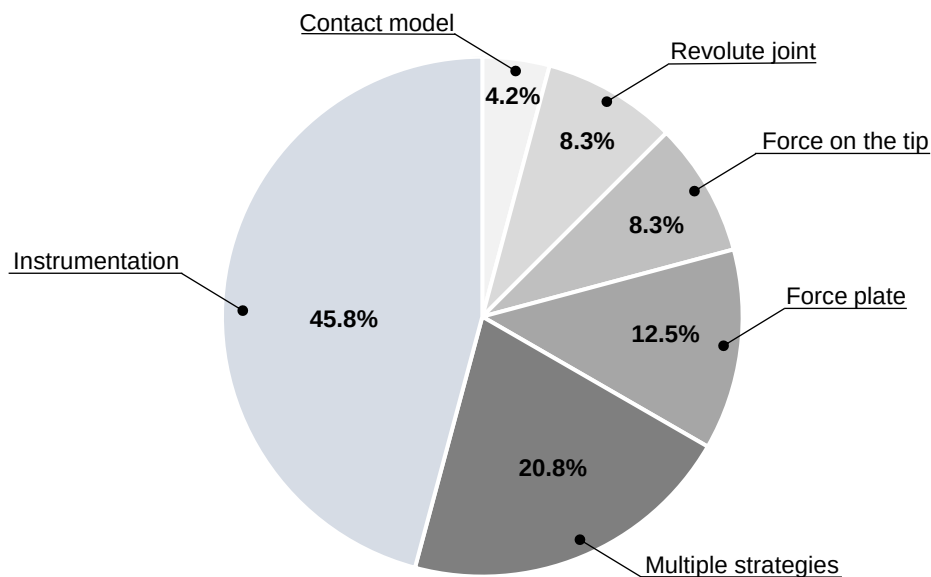


Figure 2.9 – Distribution of the approaches for crutch-ground interface considered in the studies included in this section.

2.4. Modeling the Foot-Ground Interaction

Over the last decades, the research on contact-impact modeling and analysis in multibody dynamics has received a lot of attention (Flores, 2022). However, it is still a quite challenging problem to accurately represent the contact mechanics when the geometric and material properties are of complex natures, such as in the case of the human foot-ground interface. Contact-impact events are multifaceted phenomena as the modeling process is strongly dependent on several factors, such as, the geometry of the contacting surfaces, the local physical properties, and the numerical representation of the interaction between the contacting bodies. A contact problem in multibody dynamics involves the consideration of

three main steps, namely: (i) the definition of the geometric properties of the contacting surfaces; (ii) the development of a contact search methodology; (iii) the evaluation of the contact forces resulting from the collision (Flores, 2022; Moreira et al., 2009). The contact detection is an important task in the contact modeling process, and it is related to the verification of whether the surfaces are in contact, as the relative interpenetration of the bodies is allowed. The complexity of the contacting surfaces, the number of potential contact zones, and the contact kinematics influence the accuracy and efficiency of the contact detection procedure. This is one of the most time-consuming tasks, independently of the solver utilized to mimic the physics of the contact process (Flores, 2022).

Contact-impact events have a substantial influence on the dynamic response of multibody systems, due to vibration, load propagation, deformations at the contact zone, energy dissipation, among other features that can limit the operation of the system (Flores, 2022; Skrinjar et al., 2018). In particular, the dynamic simulation of the human motion is conditioned by the foot-ground contact forces (Winter, 2009), in the measure that the response of muscles, ligaments and articular reaction forces and moments is affected by them (Shourijeh & McPhee, 2015). The human gait analysis requires the experimental evaluation of the ground reaction forces in order to provide a complete and accurate description of the human performance. However, the measurement and data acquisition of the ground reaction forces are constrained in the number of human steps, since the experimental apparatus and platforms have limited lengths. With the purpose to overcome this drawback, formulations to mimic the human foot-ground interaction have been proposed, which provide numerical approaches to calculate the ground reaction forces without the need of any experimental measurement (Moreira et al., 2009; Van Hulle et al., 2020).

The contact models, particularly those that describe the human foot-ground interaction, play a key role in biomechanical dynamic simulations. As a general classification, the available methods can be divided into “contact force” based approaches, and techniques based on “geometrical constraints”. The first method assumes that the bodies are locally deformable and establishes a physical relation between the contact forces and the foot-ground kinematics. The second method considers truly rigid contacting bodies and establishes the interaction between the foot and the ground using kinematic constraints, which change during the different phases of the gait cycle (Febrer-Nafria et al., 2018; Flores, 2022).

Regardless of the high number of research works on the foot-ground contact in the context of biomechanics of human motion, it is of paramount importance to comprehensively review the available approaches in order to allow their comparison. This has been the main motivation for this section, which permits a detailed analysis, discussion, and summary of the key features of the computational strategies to mimic the foot and ground contact interaction available in the literature.

The search approach adopted in this section was carried out on September 20, 2021. The search strategy was performed using the Boolean operators AND/OR and combined the following list of keywords

SET 1: “biomechanical model” OR “musculoskeletal model” OR “musculo-skeletal model”

SET 2: “contact model” OR “force model” OR “foot-ground contact” OR “foot-ground interaction” OR “contact forces” OR “contact detection”

Search strategy: SET 1 AND SET 2

An example of the search strategy for the case of the PubMed database is presented in Table 2.6.

Table 2.6 – Example of the search strategy for the PubMed database utilized to find the methodologies to model the foot-ground interaction in human locomotion

Search number	Terms utilized	Results
#1	biomechanical model [Title/Abstract]	1857
#2	musculoskeletal model [Title/Abstract]	1030
#3	musculo-skeletal model [Title/Abstract]	40
#4	1 OR 2 OR 3	2894
#5	contact model [Title/Abstract]	397
#6	force model [Title/Abstract]	357
#7	foot-ground contact [Title/Abstract]	122
#8	foot-ground interaction [Title/Abstract]	28
#9	contact forces [Title/Abstract]	1357
#10	contact detection [Title/Abstract]	158
#11	5 OR 6 OR 7 OR 8 OR 9 OR 10	2368
#12	4 AND 11	178

In this section, articles that include the development and/or use of a biomechanical model and incorporate the development and/or use of a human foot-ground contact modeling strategy are identified and included in the final list of analyzed papers. Apart from the exclusion criteria defined in section 2.1, the publications were excluded if (i) they did not include foot-ground contact models; (ii) the foot-ground contact model was already established in a previous publication; (iii) they utilized finite element analysis.

Database search provided a total of 900 papers, 178, 405 and 317 of which were retrieved from the PubMed, Scopus and Web of Science databases, respectively. After duplicates removal, 497 papers were screened, and 43 full-texts were retrieved to be analyzed. From this stage, 13 articles met the eligibility criteria. Seventeen additional records were identified through the careful analysis of the lists of references of the 43 full-text articles assessed for eligibility. Finally, a total of 30 papers, dated from 1995 to 2020, were included and analyzed in this section. The complete selection process is illustrated in Figure 2.10.

The full-text of all included articles in this section was analyzed, and the most significant information of the human foot-ground interaction was extracted and transferred into a customized table, which includes

the identification of both the contact geometry and the formulation of the developed and/or utilized contact model (see Table 2.7). This set of characteristics was selected to provide a comprehensive overview of the methodology developed in each article, which allows to discuss the obtained results. When the original paper provided partial information only, its list of references and the authors' previous publications were analyzed.

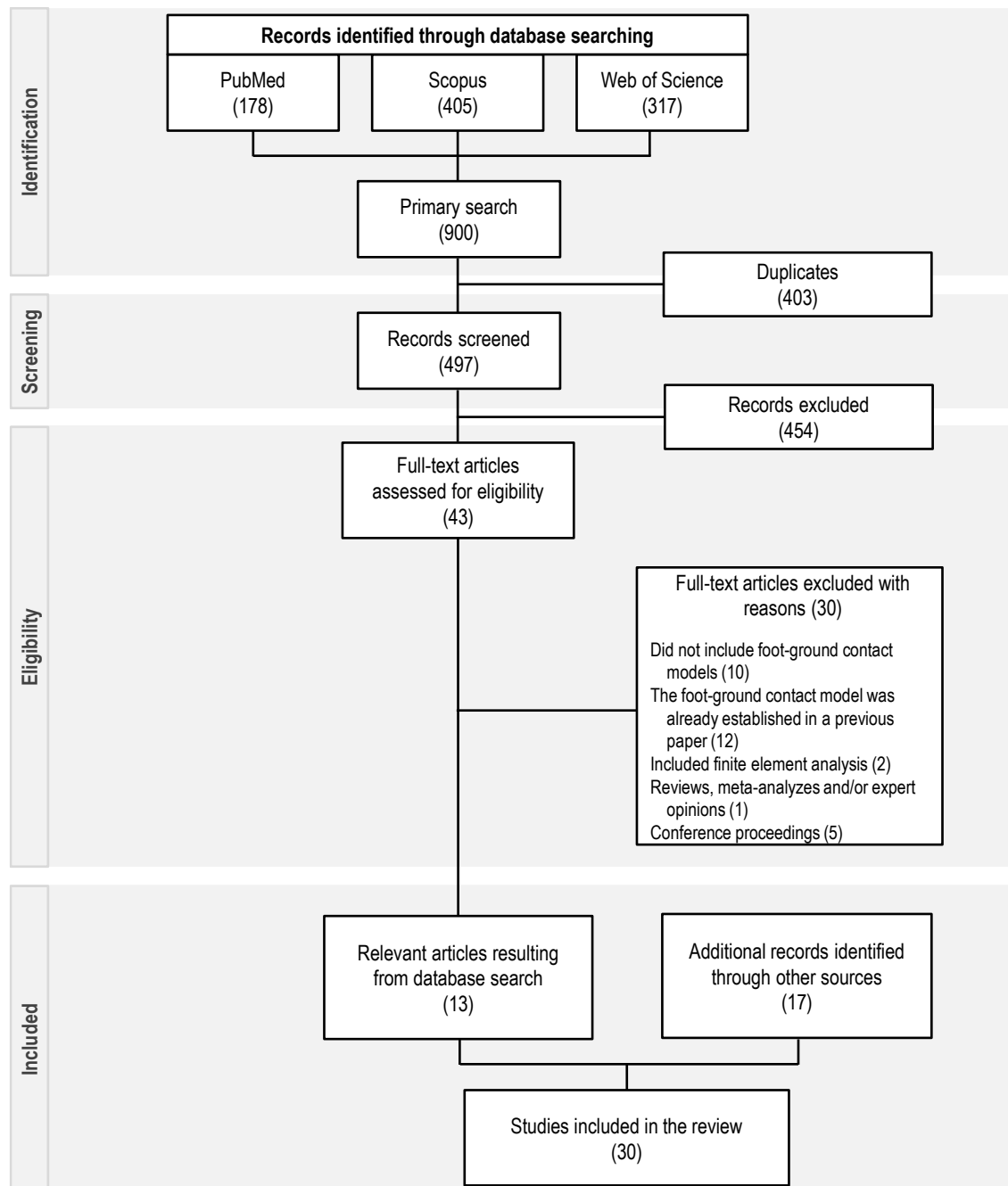


Figure 2.10 – Flowchart of the methodology conducted in this section to find studies incorporating the development and/or use of a human foot-ground contact modeling strategy.

The main goal of this section is to report and analyze the solutions available in the literature commonly utilized to study the foot-ground interaction problem in human locomotion. Figure 2.11 depicts the appearance of the 30 studies included in the present section over the years, classified according to

the total number of studies and the cumulative number of studies. It can be observed that the interest in studying the human foot-ground interaction problem has been increasing, with the period of [2015-2019] being the one with the highest number of published studies. It is important to note that only one study has been published in the period [2020-2021].

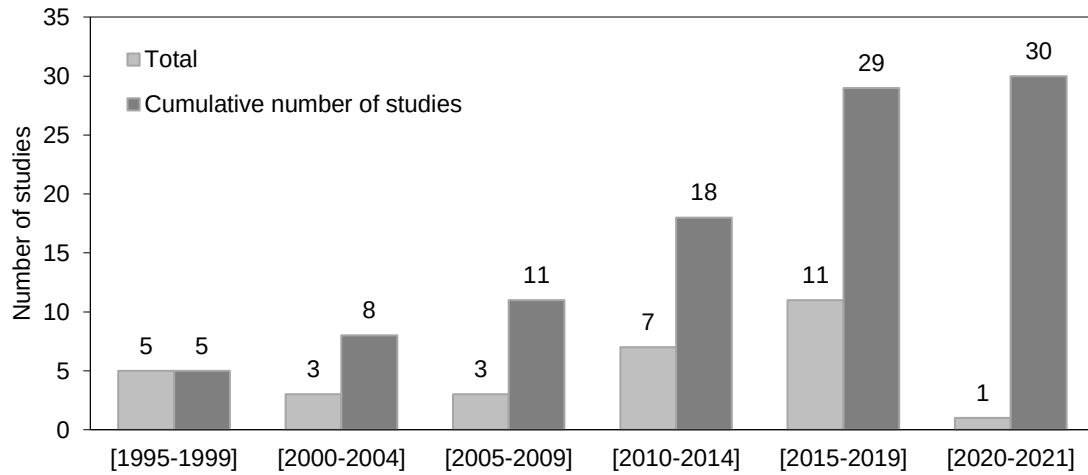


Figure 2.11 – Evolution of the number of studies on the foot-ground interaction over the years.

The main characteristics of the human foot-ground contact models are presented in Table 2.7.

Table 2.7 – Characteristics of the foot-ground contact models employed in the studies included in this section

Author, Year	Contact geometry	Contact model
Gerritsen et al. (1995)	Dimension: 2D 2 points positioned at the heel and toe	Normal GRF: nonlinear viscoelastic element $f_z = k\delta^3(1 + c\dot{\delta})$ Tangential GRF: Coulomb friction law $f_x = -\mu f_z \text{sign}(v_x)$
Gilchrist & Winter (1996)	Dimension: 3D 9 contact points arranged along the midline of the foot: 6 under the plantar surface of the foot and 3 under the toes	Normal GRF: linear spring-damper elements $f_z = k\delta + c\dot{\delta}$ where the damping coefficient is given by $c = \begin{cases} 0 & \text{if } \delta \leq 0 \\ c_{\max} \left(3 \left(\frac{\delta}{\delta_{\max}} \right)^2 - 2 \left(\frac{\delta}{\delta_{\max}} \right)^3 \right) & \text{if } 0 < \delta < \delta_{\max} \\ c_{\max} & \text{if } \delta \geq \delta_{\max} \end{cases}$ where $\delta_{\max}$ corresponds to the deformation at which the maximum damping coefficient $c_{\max}$ is achieved Tangential GRF: 2 linear dampers associated with each vertical force element
Kepple et al. (1997)	Dimension: 3D 1 point under the foot (CoP)	Normal GRF: $\delta = 0$, non-penetrating constraint Tangential GRF: $v_x = 0$, anteroposterior no-slip constraint $v_y = 0$, mediolateral no-slip constraint

Güler et al. (1998)	Dimension: 2D 1 sphere/circle at the heel pad	Normal GRF: A series of uniformly distributed Kelvin elements was considered, and the total vertical force is obtained through the integral of pressure over the contact area as $f_z = \pi k (R\delta^2 - \delta^3/3) (\delta / \delta_0)^n + \pi c (\dot{\delta} (2R\delta - \delta^2)) (\delta / \delta_0)^m$ where δ_0 is the thickness of the heel pad soft tissue and R expresses the radius of the sphere at the heel pad
F. Anderson & Pandy (1999)	Dimension: 3D 5 discrete points: 4 located at the corners of each hindfoot segment, and 1 positioned at the distal end of the toes	Normal GRF: viscoelastic elements in which the spring force varies exponentially $f_z = 0.5336e^{1150(\delta+\delta_0)} + 1000\dot{\delta}g$ $g(\delta) = \frac{1}{1+10e^{-500(\delta+g_0)}}$ where g is a function that increases the damping as the foot approaches the ground and, δ_0 and g_0 define when the magnitude of spring and damping forces, respectively, become significant Tangential GRF: linear spring-damper elements $f_x = 6.9 \times 10^4 (x - x_0) - 1000v_x$ $f_y = 6.9 \times 10^4 (y - y_0) - 1000v_y$ where x_0 and y_0 denote the rest position of the spring
Neptune et al. (2000)	Dimension: 3D 66 discrete elements attached to the foot describing the 3D exterior surface of the shoe	Normal GRF: nonlinear viscoelastic elements $f_z = A_1 (c_1 \delta^{c_2} + c_3 \delta^{c_4} \dot{\delta}^{c_5})$ where c_1, c_2, c_3, c_4 and c_5 are shoe-specific parameters and A denotes the relative element area scaling factor Tangential GRF: smoothed Coulomb friction law $f_x = \begin{cases} A_1 c_6 v_x & \text{if } A_1 c_6 v_x \leq \mu f_z \\ -\mu f_z \text{sign}(v_x) & \text{if } A_1 c_6 v_x > \mu f_z \end{cases}$ where c_6 is the viscous damping coefficient for low sliding velocities
Hase & Yamasaki (2002)	Dimension: 3D 4 points in each foot: 2 at the heel and 2 at the toe	Normal GRF: linear spring-damper elements $f_z = k\delta + c \max(\dot{\delta}, 0)$ Tangential GRF: linear spring-damper elements $f_x = -k(x - x_0) - cv_x$ $f_y = -k(y - y_0) - cv_y$ where x_0 and y_0 denote the rest position of the spring
Günther & Ruder (2003)	Dimension: 2D 3 contact points on each segment	Normal GRF: nonlinear viscoelastic element $f_z = k\delta^3 + c\delta^3 \dot{\delta}$ Tangential GRF: modeling of both adhesion and sliding states through viscoelastic element and Coulomb friction $f_x = \begin{cases} -k_x (x - x_0) x - x_0 - c_x v_x (x - x_0)^2 & \text{if adhesion} \\ \mu f_z \text{sign}(v_x) & \text{if sliding} \end{cases}$ where x_0 is the rest position of the spring The contact starts in adhesion state and changes to sliding if the following conditions are reached $ f_x > \mu_s f_z$ and $v_x > v_0$ and returns to the adhesion state if $v_x < v_0$
Peasgood et al. (2007)	Dimension: 2D 2 contact points: at the heel and ball	Normal GRF: nonlinear viscoelastic element $f_z = k\delta^n + c \min(\delta/\delta_{\max}, 1) \dot{\delta}$ where $\delta_{\max}$ is the penetration when the damping is maximum Tangential GRF: Coulomb friction law with static friction $f_x = \begin{cases} -\mu_s f_z \text{sign}(v_x) & \text{if } v_x \leq v_0 \\ -\mu_d f_z \text{sign}(v_x) & \text{if } v_x > v_0 \end{cases}$

Liu et al. (2008)	Dimension: 3D 1 point under the foot	The foot-ground interaction was modeled using spring-damper elements introduced between the feet and the floor surfaces
Goldberg & Kepple (2009)	Dimension: 3D 1 point under the foot	The model was constrained so that each foot was fixed to the ground during foot flat. After heel-off, each foot was allowed to rotate about a mediolateral pin joint passing through the center of pressure
Hamner et al. (2010)	Dimension: 3D 1 point under the foot	Normal GRF: $\delta = 0$, non-penetrating constraint Tangential GRF: $v_x = 0$, anteroposterior no-slip constraint $v_y = 0$, mediolateral no-slip constraint $\omega_z = 0$, no-twist constraint where ω_z is the foot angular velocity around the superoinferior direction
Miller et al. (2012)	Dimension: 2D 3 contact elements per foot: under heels, toe tips and metatarsophalangeal joints	Normal GRF: nonlinear viscoelastic elements $f_z = k\delta^3 e^{c\dot{\delta}}$ Tangential GRF: smoothed Coulomb friction law $f_x = -\mu f_z \tanh(v_x/v_0)$
Ackermann & van den Bogert (2012)	Dimension: 2D 10 contact points uniformly distributed along each foot sole	Normal GRF: nonlinear viscoelastic elements $f_z = k\delta^3 (1 + c\dot{\delta})$ Tangential GRF: smoothed Coulomb friction law $f_x = -\frac{1 - e^{-v_x/v_0}}{1 + e^{-v_x/v_0}} \mu f_z$
Guess et al. (2014)	Dimension: 3D Geometry of the shoe was estimated from the provided shoe size and from images of the shoe type	Normal GRF: nonlinear viscoelastic elements $f_z = k\delta^{3/2} + c\dot{\delta}$ where the damping coefficient is given by $c = \begin{cases} 0 & \text{if } \delta \leq 0 \\ c_{\max} \left(3 \left(\frac{\delta}{\delta_{\max}} \right)^2 - 2 \left(\frac{\delta}{\delta_{\max}} \right)^3 \right) & \text{if } 0 < \delta < \delta_{\max} \\ c_{\max} & \text{if } \delta \geq \delta_{\max} \end{cases}$ where $\delta_{\max}$ corresponds to the deformation at which the maximum damping coefficient $c_{\max}$ is achieved Tangential GRF: Coulomb friction law
Kia et al. (2014)	Dimension: 3D The right shoe geometry was divided into 90 pieces The left shoe was divided into heel, midfoot, and toe regions	Normal GRF: viscoelastic contact model $f_z = k\delta + c\dot{\delta}$ The damping coefficient is given by: $c = \begin{cases} 0 & \text{if } \delta \leq 0 \\ c_{\max} \left(3 \left(\frac{\delta}{\delta_{\max}} \right)^2 - 2 \left(\frac{\delta}{\delta_{\max}} \right)^3 \right) & \text{if } 0 < \delta < \delta_{\max} \\ c_{\max} & \text{if } \delta \geq \delta_{\max} \end{cases}$ where $\delta_{\max}$ corresponds to the deformation at which the maximum damping coefficient $c_{\max}$ is achieved Tangential GRF: Coulomb friction law
Jansen et al. (2014)	Dimension: 3D 3 spheres attached to the calcaneus: 1 at the heel and 2 at the metatarsal arch	The foot-ground contact was described by an elastic foundation model, in which the rigid bodies are assumed to be covered by thin elastic layers that are represented by a mesh of parallel springs, neglecting the damping component

Fluit et al. (2014)	Dimension: 3D 12 contact points under each foot: at the medial and lateral side of the heel, at the base of the first and fifth metatarsal bone, at the head of each metatarsal bone and at the big, second and fifth toe	Normal GRF: Each actuator generates a reaction force if the contact point is close enough to the ground and almost without motion $f_z = \begin{cases} qf_{\max} & \text{if } \delta > \delta_0 \text{ and } \ \mathbf{v}\ < v_0 \\ 0 & \text{otherwise} \end{cases}$ where $f_{\max}$ represents the actuator strength, q is the activation level of each actuator and δ_0 is the threshold deformation To prevent discontinuities in the estimated GRF and GRM during the transitions, a fixed time step of 0.01 s and a smoothed strength function during 12 steps were considered as $f_z = \frac{1}{2} qf_{\max} \left(1 \pm \cos\left(\frac{\pi n}{12}\right) \right) \text{ with } n = 1, \dots, 12$ Tangential GRF: A similar model is used to estimate the tangential forces f_x and f_y
Shourijeh & McPhee (2015)	Dimension: 2D Model 1: 3-point contact elements Model 2: 3 spherical/circular contact elements Model 3: 3 spherical/circular contact elements The elements are located at the heel, metatarsal joints, and toes for the three models	Normal GRF: Model 1: nonlinear viscoelastic elements $f_z = k\delta^n (1 + c\dot{\delta})$ Model 2: linear volumetric contact model $f_z = kV(1 + c\dot{\delta})$ where V is the interpenetration volume Model 3: nonlinear volumetric contact model $f_z = kV^n + cV\dot{\delta}$ where exponent n depend on the volumetric stiffness and geometrical properties and V is the interpenetration volume Tangential GRF: smoothed Coulomb friction law equal for the three models $f_x = -\mu f_z \arctan(v_x/v_0)$
Miller & Hamill (2015)	Dimension: 2D 11 contact elements spaced evenly from heel to toe tip	Normal GRF: nonlinear viscoelastic elements $f_z = k\delta^2 (1 + c\dot{\delta})$ Tangential GRF: smoothed Coulomb friction law $f_x = -\mu f_z \tanh(v_x/v_0)$
Lopes et al. (2016)	Dimension: 3D Model 1: 31 points distributed over the three foot segments describing the shoe's profile Model 2: 6 ellipsoid-plane contact pairs, rigidly attached to the three foot segments	Both models utilize a continuous contact force law that considers the minimum distance and relative velocities between two potential contacting surfaces The contact force model was the same as in Neptune et al. (2000)
Jung et al. (2016)	Dimension: 3D Model 1: 40 points attached to the sole of the foot Model 2: 1 point attached to the center of pressure on the sole of the foot	Model 1: the maximum force of the reaction components was adjusted according to the vertical displacement and anteroposterior velocity $f = 500d_f s_f$ where d_f is the vertical displacement factor and s_f is the speed factor $d_f = \begin{cases} 0 & \text{if } \delta \leq \delta_0 \\ 1 - \delta/\delta_0 & \text{if } \delta_0 < \delta < 0 \\ 1 & \text{if } \delta \geq 0 \end{cases} \quad s_f = \begin{cases} 0 & \text{if } v_x \geq v_0 \\ 1 - v_x/v_0 & \text{if } v_0 < v_x < 0 \\ 1 & \text{if } v_x \leq 0 \end{cases}$ Model 2: the reaction force between the CoP and ground was adjusted to match the vertical GRF according to Coulomb's law and was activated when the vertical GRF was greater than a threshold value $f_{x,\max} = \begin{cases} 0 & \text{if } f_z < f_0 \\ f_z & \text{if } f_z > f_0 \end{cases}$

Meyer et al. (2016)	Dimension: 3D 11 (anteroposterior) × 8 (mediolateral) grid of rectangular contact elements	Normal GRF: linear spring with nonlinear damping $f_z = k(\delta - \delta_0)(1 + c\dot{\delta})$ where δ_0 is the spring resting length common to all springs on the same foot and essentially adjusts the height of the ground Tangential GRF: smoothed Coulomb friction law $f_x = -\mu f_z \tanh(v_x/v_0)$
Lin & Pandy (2017)	Dimension: 3D 6 spheres placed under the foot – 4 at the hindfoot and 2 at the toes	The contact force model was the same as in Miller & Hamill (2015)
Brown & McPhee (2018)	Dimension: 3D 3 ellipsoids: 2 at the hindfoot (1 for the heel and 1 for the ball), and 1 at the toe segment	Normal GRF: linear volumetric contact model $f_z = kV(1 + c\dot{\delta})$ where V is the volume of penetration Tangential GRF: smoothed friction model with static friction $f_x = - \left[\mu_d \tanh\left(4 \frac{v_x}{v_0}\right) + (\mu_s - \mu_d) \frac{\frac{v_x}{v_0}}{\left(\frac{1}{4} \left(\frac{v_x}{v_0}\right)^2 + \frac{3}{4}\right)^2} \right] f_z \text{sign}(v_x)$
Razu & Guess (2018)	Dimension: 3D The shoe geometry was obtained by 3D scanning shoes	The shoe-ground interface was modeled using compliant contacts between the shoe and force plates, which were represented by a simple box
Dorschky et al. (2019)	Dimension: 2D 2 contact points placed at the heel and ball	Normal GRF: polynomial function of the deformation to fit the measurement data $f_z = k_1 d + k_2 d^2 + k_3 d^3 + c d \dot{\delta}$ where k_1, k_2, k_3 are the stiffness parameters and d is the penetration smoothed for a continuous and differentiable function as $d = \frac{1}{2}(\sqrt{\delta^2 + \delta_0^2} + \delta)$ where δ_0 is the tolerance deformation to smooth force transition Tangential GRF: smoothed Coulomb friction law $f_x = -\mu f_z \frac{v_x}{\sqrt{v_x^2 + v_0^2}}$
Moissenet et al. (2019)	Dimension: 3D 1 fixed contact point was defined on the forefoot	The acceleration and velocity of the contact point was constrained to be null $\mathbf{C}(\mathbf{q})\ddot{\mathbf{q}} + \dot{\mathbf{C}}(\mathbf{q})\dot{\mathbf{q}} = \mathbf{0} \text{ and } \mathbf{C}(\mathbf{q})\dot{\mathbf{q}} = \mathbf{0}$ where $\mathbf{C}$ is the external contact Jacobian matrix and $\mathbf{q}, \dot{\mathbf{q}}$ and $\ddot{\mathbf{q}}$ are the generalized positions, velocities, and accelerations, respectively
Millard & Mombaur (2019)	Dimension: 2D Model 1: ellipse-foot (a single-segment foot) Model 2: double-circle foot (a two-segment foot)	Model 1: the constraints between the ellipse and the plane are applied at the closest point and are described at the velocity-level $v_z^s = 0 \text{ and } v_x^s = 0$ (contact and no-slip constraints) where v_x^s and v_z^s are the anteroposterior and superoinferior velocities of the ellipse point closest to the ground, respectively Model 2: one of three different sets of constraint equations depending on the contact case

		Heel contact: $v_z^H = 0$ and $v_x^H = 0$ (contact and no-slip constraints) Forefoot contact: $v_z^F = 0$ and $v_x^F = 0$ (contact and no-slip constraints) Both heel and forefoot touch the ground: the contact constraint is applied to both points ($v_z^H = 0$ and $v_z^F = 0$), while the no-slip constraint is just applied to one of them ($v_x^H = 0$ or $v_x^F = 0$) where H and F refer to the heel and forefoot contact points, respectively
Van Hulle et al. (2020)	Dimension: 2D Model 1: 3 control points are placed on the foot at the ground level based on experimental markers Model 2: a contact point is determined, which represents the center of pressure	Model 1: non-penetration and non-slipping condition at three control points Model 2: Normal GRF: unilateral constraint at the point representing the CoP, with a non-penetration condition in a form of a complementarity problem: $g \geq 0, f_z \geq 0, g f_z = 0$ where g is the distance between the point and the ground Tangential GRF: no-slip constraint at the point representing the CoP as if $g = 0$ then $\Delta x = 0$ else $f_x = 0$ where g is the distance between the point and the ground and Δx denotes the tangential displacement

The contact geometry varied substantially across studies. The simplest models considered a single point of contact between the human foot and the ground, generally representing the center of pressure (CoP). This is the case of Kepple et al. (1997), Liu et al. (2008) and Goldberg & Kepple (2009). The consideration of only one contact point is a simple approach to deal with the human foot-ground interaction problem. Therefore, in order to increase the reliability of the model, other studies utilized more than one point. As examples, the works of Gerritsen et al. (1995), Ackermann and van den Bogert (2012), and Miller & Hamill (2015) fall within this category, as they considered 2, 10 and 11 contact points, respectively. However, this approach is still not representative of a natural human foot shape. In this regard, other models have considered more complex geometries, such as circles, ellipses, spheres, or ellipsoids, which intend to better capture the actual human foot surface geometry. The works of Güler et al. (1998), Lin & Pandy (2017), and Brown & McPhee (2018) are examples of models including those geometric characteristics. Contact geometries described by surfaces have higher accuracy and provide improved reliability than point contact models, since they provide a wider contact area and, therefore, result in the calculation of smoother contact forces (Shourijeh & McPhee, 2015). There are studies that compare different human foot-ground interaction geometries in order to assess which one provides better solutions for this problem. For instance, Shourijeh & McPhee (2015) evaluated three different models, consisting of three contact points, spheres or circles located at the heel, metatarsal joints, and toes, respectively. It was observed that the point contact model is not an accurate representation of the human

foot-ground contact during gait, as there is no smooth transition between the variations in the contact force. This study concluded that the transition from a contact point model to a model defined by spheres or circles presented a promising progress in the generation of contact forces in agreement with experimental data (Shourijeh & McPhee, 2015). Moreover, Lopes et al. (2016) compared two different geometries for the contact model, one composed of 31 points of contact attached beneath the foot in locations that described the profile of the shoe, and another consisting of six ellipsoids fixed on the foot and placed within the shoe's boundary. The conclusion was that the ellipsoid elements were more versatile and geometrically accurate than points, since point models have discrete spatial resolution, while surface models have continuous spatial resolution and allow volumetric contact during three-dimensional motions. Guess et al. (2014), Kia et al. (2014), and Razu & Guess (2018) considered 3D scanning procedures, which allows the definition of a more anatomically accurate contact geometry.

Figure 2.12 depicts the number of studies according to the considered contact geometry. Due to their geometric simplicity, a significant number of studies utilized point elements. The accuracy of this type of contact geometry depends on the number of included elements and their distribution along the foot. On the one hand, increasing the number of point elements benefits the biofidelity of the model, but also raises the number of calculations required and penalizes the computational efficiency. On the other hand, reducing the number of points increases the model's stiffness, which also negatively affects its computational efficiency. Surface approaches enhance the computational efficiency due to the use of a reduced number of elements to define the contact when compared with point approaches, as a single surface can represent an infinite set of points. The contact geometry must produce good results in terms of contact forces and provide a good computational efficiency. In this perspective, superellipsoid contact elements seem to be an interesting solution, as they characterize general-purpose shape models and encompass spherical, ellipsoidal, and cylindrical shapes altogether into a single mathematical expression.

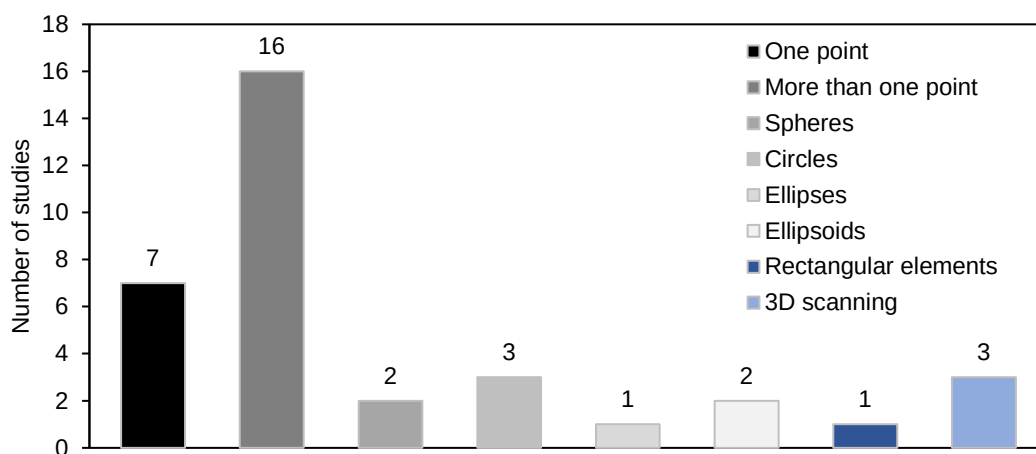


Figure 2.12 – Number of studies organized according to the contact geometry for the foot-ground interaction model.

The majority of studies (77%) utilized contact force approaches. For instance, Güler et al. (1998) used viscoelastic spheres to model the heel pad using Kelvin elements, considering both stiffness and damping properties. Also, the vertical ground reaction forces were modeled as a nonlinear spring-damper arrangement positioned vertically at the heel and toes of the foot in Gerritsen et al. (1995). Contact force approaches are simple, straightforward to implement and, generally, computationally efficient. However, the difficult selection of appropriate contact parameters to introduce into the model is a general drawback of this approach. In addition, due to the presence of stiff springs on the compliant surfaces to model the contact, force models may introduce high-frequency dynamics into the system, which may require smaller steps in the integration algorithm, penalizing the computational efficiency. It is important to note that one of the contact models provided in the study of Jung et al. (2016) (Model 2) only estimates the tangential ground reaction forces, since the vertical ground reaction force and the location of the center of pressure are obtained experimentally. Alternatively, in only 23% of studies, the human foot-ground contact problem was based on geometric constraints. For example, Hamner et al. (2010) modeled the interaction between the foot and the ground using a combination of a non-penetrating unilateral constraint and a pure rolling constraint. This approach assumes that the contacting bodies are truly rigid, in contrast to the assumption of locally deformable bodies considered in contact force approaches. This formulation uses the unilateral constraints to compute contact impulses or forces to prevent penetration from occurring (Flores, 2022).

2.5. Summary and Discussion

This chapter presents an overview of the literature on topics related to biomechanical modeling of device-assisted locomotion. Initially, the characteristics of biomechanical systems utilized to study locomotion aided by four types of assistive devices, namely, crutches, walkers, wheelchairs, and canes, were reviewed. The majority of studies utilized 3D models, and unilateral upper extremity models were preferred over full-body or bilateral upper extremity models. The modeling of the upper extremity is still very simplified, as very few studies include detailed representations of the upper limb joints and segments. It was concluded that the interest for crutch-assisted locomotion modeling has been rising over the years, which laid the basis for a deeper literature review on this topic. Several strategies were found for incorporating crutches into models, along with the approaches utilized to deal with the interactions of this assistive device with the ground and human body. The available methodologies to study the foot-ground interaction were also reviewed. It was found that the most common geometries were based on points. Regarding the resolution of the foot-ground interaction, the formulations based on contact force approaches were preferred to the methods based on geometrical constraints.

"It does not matter how slowly you go as long as you do not stop."

Confucius

3. MULTIBODY SYSTEMS WITH CARTESIAN COORDINATES

The dynamic analysis of multibody systems has an extensive potential of application in a broad variety of engineering areas of investigation. In the specific domain of biomechanics of motion, multibody dynamics has emerged as a vital and widely employed approach for investigating and understanding the movement and the dynamic response of the human body in diverse real-world scenarios. The formulation of multibody systems dynamics adopted in the present work closely follows that of Nikravesh (1998), in which the generalized Cartesian coordinates and the Newton-Euler's formulation are employed to derive the equations of motion of the systems. Additionally, the Baumgarte stabilization technique is considered in order to control the position and velocity violations. The multibody systems formulation allows for the three-dimensional analysis of multibody models, and it constitutes the foundation for the description and development of the biomechanical systems implemented in this work. In the beginning of this chapter, an introduction to the methodologies underlying the dynamic analysis of multibody systems is provided. Afterwards, the formulations developed in this work are thoroughly explained and described, namely the proposed modified universal joint, the improved methodology to restrict the range of motion of mechanical joints and the driving constraints formulation. This chapter ends with three application examples incorporating all the approached concepts.

3.1. Introduction to Multibody Systems Methodologies

Multibody dynamics is a powerful tool for the systematic simulation, analysis, and optimization of the motion of mechanical systems and it has a vast spectrum of application in several engineering areas, including biomechanics of motion. In a simple manner, it can be said that a general multibody mechanical system is composed of three main ingredients, i.e., a collection of rigid and/or deformable bodies describing large rotational and translational motions, joints kinematically constraining the relative motion of the bodies, and force or driving elements acting upon those bodies (Flores, 2015; P. Nikravesh, 1988). Figure 3.1 depicts a schematic abstract representation of a general multibody mechanical system.

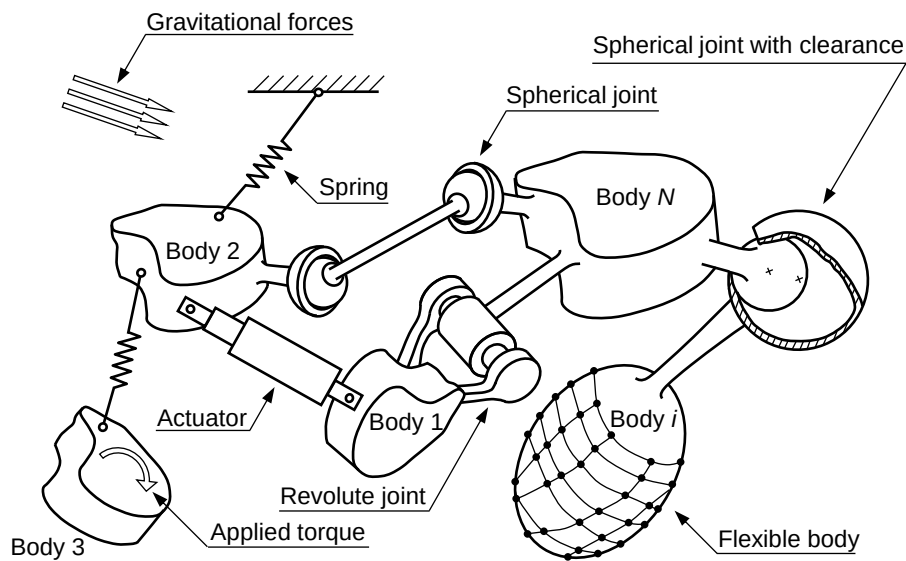


Figure 3.1 – Schematic abstract representation of a general multibody mechanical system including the most representative elements, namely bodies, joints, and forces.

In this work, the bodies of the multibody systems are assumed to be rigid, which is a reasonable modeling option as their deformations do not have a significant impact on the response of the system. For spatial systems, each rigid body has six degrees-of-freedom, namely three translations and three rotations. When a mechanical joint is introduced into a multibody system, the number of degrees-of-freedom is reduced since the joint is responsible for constraining the relative motion between the connected bodies. Depending on the relative degrees-of-freedom allowed, the joints can be classified as revolute, translational, spherical, universal joints, among others (Flores, 2015; P. Nikravesh, 1988). According with the purpose of the analysis, the joints can be considered as ideal or imperfect. Ideal joints impose kinematic relations between the connected bodies, while imperfect joints intend to reproduce realistic phenomena, including, for instance, clearance, friction, or lubrication. In this work, ideal joints are utilized. The kinematic constraint equations utilized to mathematically describe ideal joints can be classified as holonomic or nonholonomic constraints, depending on whether or not they are integrable into a form involving only coordinates, respectively. In addition, the constraints can further be classified as rheonomic or scleronomic, whether or not they are explicit functions of time, respectively (Flores, 2015; Marques, 2020).

The configuration of a multibody system can be described using different types of coordinates, namely absolute, relative, natural, or fully cartesian coordinates (Flores, 2015; P. E. Nikravesh, 2019; I. Roupá et al., 2023). In this work, absolute coordinates are considered, in which each body of the multibody system is represented by three translational and four orientational coordinates, which are known as the Cartesian coordinates. The orientational coordinates of a rigid body are the Euler parameters, which are based on the Euler's theorem on finite rotation. The theorem states that any rotation in the three-dimensional

space can be described by a rotation about a certain axis of a certain angle. Hence, the vector of generalized coordinates considered in this work for a given body i is expressed by seven coordinates as

$$\mathbf{q}_i = \{\mathbf{r}_i \ \mathbf{p}_i\}^T \quad (3.1)$$

where $\mathbf{r}_i$ is the vector of the translational coordinates of body i expressed in global coordinates as

$$\mathbf{r}_i = \{x_i \ y_i \ z_i\}^T \quad (3.2)$$

and $\mathbf{p}_i$ represents the vector of the Euler parameters (e_k , $k = 0, 1, 2, 3$) of body i given by

$$\mathbf{p}_i = \{e_0 \ e_1 \ e_2 \ e_3\}^T \quad (3.3)$$

It is important to note that the use of the Euler parameters implies four coordinates to describe the orientation of a body. However, since a constraint imposing that vector $\mathbf{p}_i$ must be a unit vector is considered, the number of independent coordinates remains three (Marques, 2020).

The generalized velocities vector of a rigid body i can be written as

$$\mathbf{v}_i = \{\dot{\mathbf{r}}_i \ \boldsymbol{\omega}_i\}^T \quad (3.4)$$

in which the dot represents the derivative with respect to time and $\boldsymbol{\omega}_i$ is angular velocity vector of body i .

The generalized accelerations vector of a rigid body i is defined by taking the time derivative of Eq. (3.4) and it is expressed as

$$\dot{\mathbf{v}}_i = \{\ddot{\mathbf{r}}_i \ \dot{\boldsymbol{\omega}}_i\}^T \quad (3.5)$$

where $\dot{\boldsymbol{\omega}}_i$ denotes the angular acceleration vector of body i .

The multibody dynamics analysis includes the development of mathematical models of the equations of motion of the systems under analysis, as well as the implementation of computational procedures to simulate, analyze, and optimize the global motion produced. For a constrained multibody system, the kinematic constraints can be described by a set of linear and/or nonlinear holonomic algebraic equations as

$$\boldsymbol{\Phi} \equiv \boldsymbol{\Phi}(\mathbf{q}, t) = \mathbf{0} \quad (3.6)$$

in which $\mathbf{q}$ is the vector of generalized coordinates of the system and t represents the time variable.

Differentiating Eq. (3.6) with respect to time yields the velocities constraint equations as

$$\dot{\boldsymbol{\Phi}} \equiv \mathbf{D}\mathbf{v} - \mathbf{v} = \mathbf{0} \quad (3.7)$$

where $\mathbf{D}$ is the Jacobian matrix of the constraint equations (3.6), $\mathbf{v}$ represents the vector of generalized velocities of the system and $\mathbf{v}$ denotes the right-hand side of the velocities constraint equations. Vector $\mathbf{v}$ is null for scleronomic constraints since it expresses the partial derivatives of $\boldsymbol{\Phi}$ with respect to time.

A second differentiation of Eq. (3.6) with respect to time leads to the acceleration constraint equations, which are established as

$$\ddot{\Phi} \equiv \mathbf{D}\dot{\mathbf{v}} - \boldsymbol{\gamma} = \mathbf{0} \quad (3.8)$$

in which $\dot{\mathbf{v}}$ is the vector of generalized accelerations of the system and $\boldsymbol{\gamma}$ represents right-hand side vector of the acceleration constraint equations. Vector $\boldsymbol{\gamma}$ contains the quadratic velocity terms and the terms that are solely function of velocity, position, and time (Flores, 2015).

Three main methodologies can be applied to derive the equations of motion of a multibody system, namely the Newton-Euler, Lagrange, and Kane methodologies. In this work, the Newton-Euler approach with absolute coordinates is adopted since it is amongst the most widely used methods in several engineering fields because it is simple, direct, and quite intuitive for general-purpose codes to model multibody systems (Flores, 2015; Marques et al., 2021). The motion of the center of mass of rigid bodies is related to the forces and moments acting upon them by the Newton-Euler equations as

$$\mathbf{M}\dot{\mathbf{v}} = \mathbf{g} + \mathbf{g}^c \quad (3.9)$$

where $\mathbf{M}$ denotes the system mass matrix, which results from the combination of the mass matrix associated with each body as

$$\mathbf{M} = \begin{bmatrix} m_1 \mathbf{I}_{3 \times 3} & \mathbf{0} & & & \\ \mathbf{0} & \mathbf{J}_1 & & & \\ & & \ddots & & \\ & & & m_i \mathbf{I}_{3 \times 3} & \mathbf{0} \\ & & & \mathbf{0} & \mathbf{J}_i \\ & & & & \ddots \\ & & & & & m_N \mathbf{I}_{3 \times 3} & \mathbf{0} \\ & & & & & \mathbf{0} & \mathbf{J}_N \end{bmatrix} \quad (3.10)$$

in which m_i is the mass of body i , $\mathbf{J}_i$ is the respective inertia tensor, $\mathbf{I}$ is the identity matrix and N is the total number of bodies of the system. Vector $\mathbf{g}^c$ of Eq. (3.9) denotes the vector of reaction forces and moments on the kinematic joints in the global coordinate system. Vector $\mathbf{g}^c$ is null in unconstrained multibody systems. Considering the Lagrange multipliers technique, vector $\mathbf{g}^c$ can be expressed as a function of the Jacobian matrix of the constraint equations and the vector of Lagrange multipliers as

$$\mathbf{g}^c = -\mathbf{D}^T \boldsymbol{\lambda} \quad (3.11)$$

where $\boldsymbol{\lambda}$ is the vector of the Lagrange multipliers that contains the reaction forces and moments on the kinematic joints. The size of vector $\boldsymbol{\lambda}$ is equal to the number of holonomic constraints, since each element is associated with the reaction force or moment imposed by each kinematic constraint (Flores, 2015).

Vector $\mathbf{g}$ of Eq. (3.9) represents the vector of external generalized forces and gyroscopic moments, expressed as

$$\mathbf{g} = \begin{Bmatrix} \mathbf{f}_1 \\ \mathbf{n}_1 - \tilde{\boldsymbol{\omega}}_1 \mathbf{J}_1 \boldsymbol{\omega}_1 \\ \vdots \\ \mathbf{f}_i \\ \mathbf{n}_i - \tilde{\boldsymbol{\omega}}_i \mathbf{J}_i \boldsymbol{\omega}_i \\ \vdots \\ \mathbf{f}_N \\ \mathbf{n}_N - \tilde{\boldsymbol{\omega}}_N \mathbf{J}_N \boldsymbol{\omega}_N \end{Bmatrix} \quad (3.12)$$

in which $\mathbf{f}$ represents the sum of the external forces acting on the origin of the body-fixed frame, $\mathbf{n}$ is the sum of external moments acting on a body, and $\tilde{\boldsymbol{\omega}}_i \mathbf{J}_i \boldsymbol{\omega}_i$ denotes the term of the gyroscopic moments.

By assembling the Newton-Euler equations of motion (3.9) and (3.11) for a constrained multibody system and the accelerations constraints equations (3.8), the governing equations for a dynamic multibody system with holonomic constraints are formulated as (P. Nikravesh, 1988)

$$\begin{bmatrix} \mathbf{M} & \mathbf{D}^T \\ \mathbf{D} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \dot{\mathbf{v}} \\ \boldsymbol{\lambda} \end{Bmatrix} = \begin{Bmatrix} \mathbf{g} \\ \boldsymbol{\gamma} \end{Bmatrix} \quad (3.13)$$

Equation (3.13) is a differential algebraic equation of index-1 and represents the equations of motion of the multibody system, which can be solved for the generalized accelerations vector and the Lagrange multipliers vector. The motion of the multibody system can be achieved by the time integration of the accelerations and determined in each time step in order to find the new positions and velocities, respectively (Marques, 2020). It is important to note that Eq. (3.13) does not explicitly include the position, $\boldsymbol{\Phi}$, and velocity, $\dot{\boldsymbol{\Phi}}$, constraint equations, which, for moderate or long simulations, results in the violation of those original constraints. In the first steps of the simulation, the constraints violations are usually small and negligible. However, for moderate or long simulations, the violation of the original constraints formulated for the problem cannot be neglected. Thus, after several simulation steps, the results might be unacceptable (Flores & Lankarani, 2016; P. Nikravesh, 1988). The constraints violation might be associated either with the integration procedures, time step selected, and/or inaccurate initial conditions. In order to overcome or minimize this problem, several strategies can be implemented, namely stabilization techniques, coordinate partitioning methods, and direct correction formulations (P. Nikravesh, 1988). In this work, the Baumgarte stabilization technique is taken into consideration, and, thus, Eq. (3.13) can be rewritten as

$$\begin{bmatrix} \mathbf{M} & \mathbf{D}^T \\ \mathbf{D} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \dot{\mathbf{v}} \\ \lambda \end{Bmatrix} = \begin{Bmatrix} \mathbf{g} \\ \gamma - 2\alpha\dot{\Phi} - \beta^2\Phi \end{Bmatrix} \quad (3.14)$$

where α and β represent the feedback control parameters for velocity and position constraint violations, respectively, and are taken as positive constants.

The first step in the standard resolution of the equations of motion deals with the definition of the initial instant of time, t_0 , and initial conditions of the system, specifically the initial positions, $\mathbf{q}_0$, and velocities, $\mathbf{v}_0$. Subsequently, the vectors γ , $\mathbf{g}$, Φ and $\dot{\Phi}$, as well as the matrices $\mathbf{M}$ and $\mathbf{D}$ are evaluated, and Eq. (3.14) is solved for the constrained multibody system in order to obtain $\dot{\mathbf{v}}$ and λ for time instant t . Then, the auxiliary vector $\dot{\mathbf{y}}_t$ for time t , which contains the velocities and accelerations of the system, is assembled and numerically integrated for time instant $t+\Delta t$ to obtain vector $\mathbf{y}_{t+\Delta t}$. Thus, the new velocities and positions of the system are obtained. In order to proceed with the simulation, the time variable must be updated after completing each time step. In this situation, if the final simulation time has not been reached yet, the simulation continues, and the previously described steps are repeated for the following time steps. This procedure continues until the final time of the analysis is reached (Flores & Lankarani, 2016). The flowchart of the computational procedure for the dynamic analysis of multibody mechanical systems is presented in Figure 3.2.

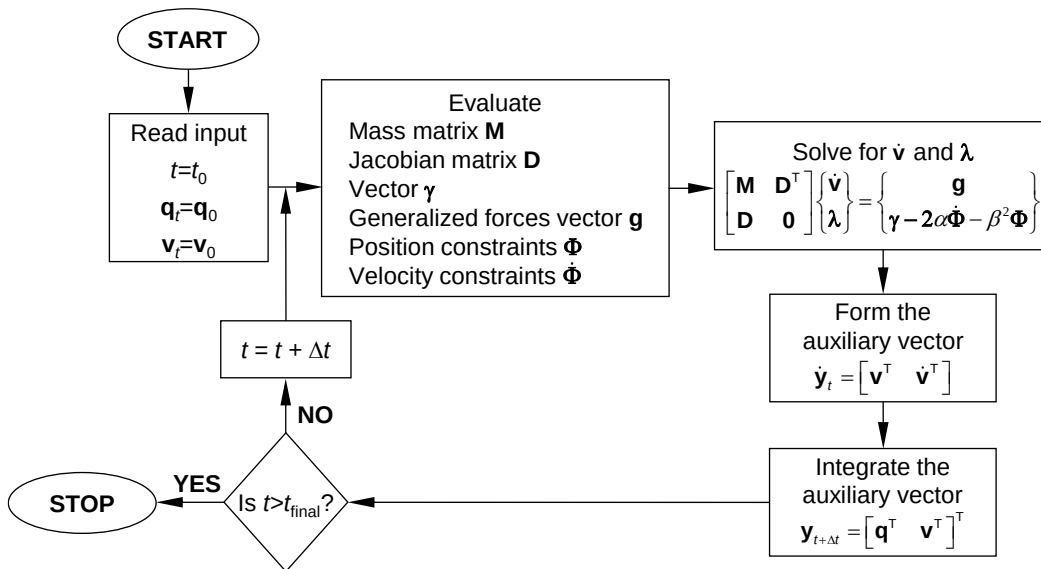


Figure 3.2 – Flowchart illustrating the computational procedure for the dynamic analysis of multibody systems based on the Baumgarte stabilization method.

Over the last decades, the use of biomechanical models to study the human movement has been increasing in many science and engineering fields (I. Roupia et al., 2022; M. Silva et al., 2021; M. R. Silva, Marques, Silva, et al., 2023), such as sports (Quental et al., 2023), clinical studies (Febrer-Nafria et al.,

2021; Lúgrís, Carlin, Luaces, et al., 2013) and crashworthiness research (Bedewi & Digges, 1999; Metzler et al., 2007). A biomechanical model is a mathematical representation of the human body and can be established using different numerical approaches, including the multibody systems methodology. The validity of the results provided by the biomechanical models is strongly dependent on their computational efficiency and anatomical accuracy, such as the reliable modeling of body segments, joints, or the body-environment interaction (Saraiva et al., 2022; M. R. Silva et al., 2022b). Integrating multibody dynamics formulations into the modeling and simulation of the human body can significantly improve the understanding of healthy and pathological movement and how it may impact clinical intervention strategies and rehabilitation procedures. The knowledge on this topic may shed light on biomechanical demands placed on the joints and can guide the development of novel assistive devices tailored to the needs of each subject, as well as type and level of disability, ultimately improving the locomotion efficiency and also end-user comfort.

3.2. Description of the Modified Universal Joint

Due to its intricate nature, the ankle joint complex of the human foot is a quite challenging problem to handle under the umbrella of biomechanics of motion discipline. The foot is the part of the human body that contacts the ground, and it comprises three major bone groups, namely, the tarsus, metatarsus, and the phalanges, as observed in Figure 3.3a (Palastanga & Soames, 2012; Standring, 2008). The tarsus group is composed of seven bones. One of them is the calcaneus, that projects posteriorly on the foot, forming the prominence of the heel. The remaining bones are the talus, the navicular, the cuboid and the three cuneiform bones, namely medial, intermediate, and lateral cuneiforms. The metatarsus group includes five different metatarsal bones, which do not have specific names, being numbered from one to five with roman numerals, starting from the medial side of the foot. Finally, there are two phalanges in the great toe (proximal and distal), while the remaining toes comprise three phalanges each (proximal, middle, and distal) (Palastanga & Soames, 2012) (see Figure 3.3a). The intricate interconnections that exist between the bones of the human foot result in the establishment of 31 articulations that allow several movements during daily life activities (Standring, 2008). Amongst these 31 articulations, the talocrural and the talocalcaneal articulations, which collectively form the ankle joint complex of the human foot (Brockett & Chapman, 2016; Fukano et al., 2018; McKeon & Hoch, 2019), are the foundation for the formulation of the modified universal joint proposed here. The talocrural articulation enables plantarflexion and dorsiflexion, and it is located between the superior surface of the talus of the foot and the distal ends of the tibia and fibula of the leg. The foot also allows inversion and eversion, which are movements

provided by the talocalcaneal articulation that is located between the tarsal bones of the posterior part of the foot, more specifically between the superior surface of the calcaneus and the inferior surface of the talus (B. Pereira et al., 2021; Standring, 2008). While the talocrural and the talocalcaneal articulations are the major contributors to plantarflexion, dorsiflexion, inversion and eversion of the foot, those movements are a result of the combination of the different degrees-of-freedom of the ankle and foot in all cardinal planes. A schematic representation of the ankle joint complex is provided in Figure 3.3b.

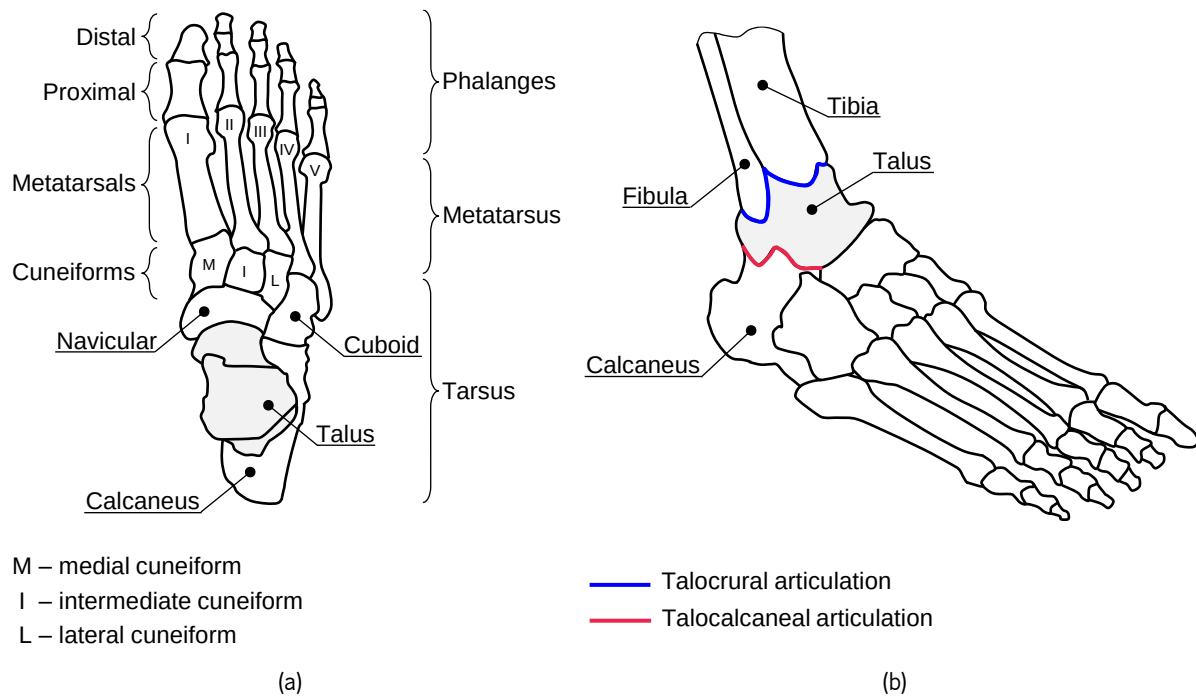


Figure 3.3 – Schematic representation of the (a) bones and (b) ankle joint complex of the right human foot.

The ankle joint complex of the human foot has two anatomical particularities. The first one is associated with the fact that the anatomical axes of the talocrural and the talocalcaneal articulations do not intersect at a specified point, but, instead, they are separated by a certain distance. Therefore, the joint axes are non-coplanar and the distance between them can be established as the length of the talus since this bone is inserted between the two articulations (see Figure 3.3b). The second particularity is that the axes of the talocrural and the talocalcaneal articulations define specific anatomical orientations between each other (F. Anderson & Pandy, 1999; Dettwyler et al., 2004; Isman & Inman, 1969; Neumann, 2013), as observed in Figure 3.4. Both the talocrural and the talocalcaneal joint axes are composed of two rotations in two cardinal planes and around two anatomical axes. In order to determine the axis of the talocrural articulation, a rotation around the superoinferior axis in the transverse plane must be completed (see Figure 3.4a), followed by a rotation around the anteroposterior axis in the frontal plane (see Figure 3.4b). For the talocalcaneal articulation, a rotation around the superoinferior axis in the transverse plane (see Figure 3.4a) is followed by a rotation around the mediolateral axis in the sagittal

plane (see Figure 3.4c). It is important to note that the angles shown in Figure 3.4 are projected onto the corresponding cardinal plane. Therefore, after the first rotation in one plane using the angle projected on that plane, the second rotation requires calculating the corresponding angle as the real angle between the transverse plane of the body and the joint axis. In order to determine the real angles, the following conditions must be utilized (see Figure 3.4) (Mott et al., 2018; Nisbett & Budynas, 2006)

$$\tan \theta_{re} = \tan \theta \cos \rho \quad (3.15)$$

$$\tan \tau_{re} = \tan \tau \cos \varepsilon \quad (3.16)$$

where the subscript 're' represents the real angle. After calculating the real angles using Eqs. (3.15) and (3.16), the talocalcaneal and the talocrural axes can be expressed, respectively, as

$$\mathbf{s}_{\text{talocalcaneal}} = \{\cos \rho \cos \theta_{re} \quad \sin \rho \cos \theta_{re} \quad \sin \theta_{re}\}^T \quad (3.17)$$

$$\mathbf{s}_{\text{talocrural}} = \{\sin \varepsilon \cos \tau_{re} \quad \cos \varepsilon \cos \tau_{re} \quad \sin \tau_{re}\}^T \quad (3.18)$$

The values of ρ , θ , ε and τ can be retrieved from F. Anderson & Pandy (1999), and express the angles of the axes of both articulations projected onto the cardinal planes when the foot stands in the anatomical reference position, as depicted in Figure 3.4.

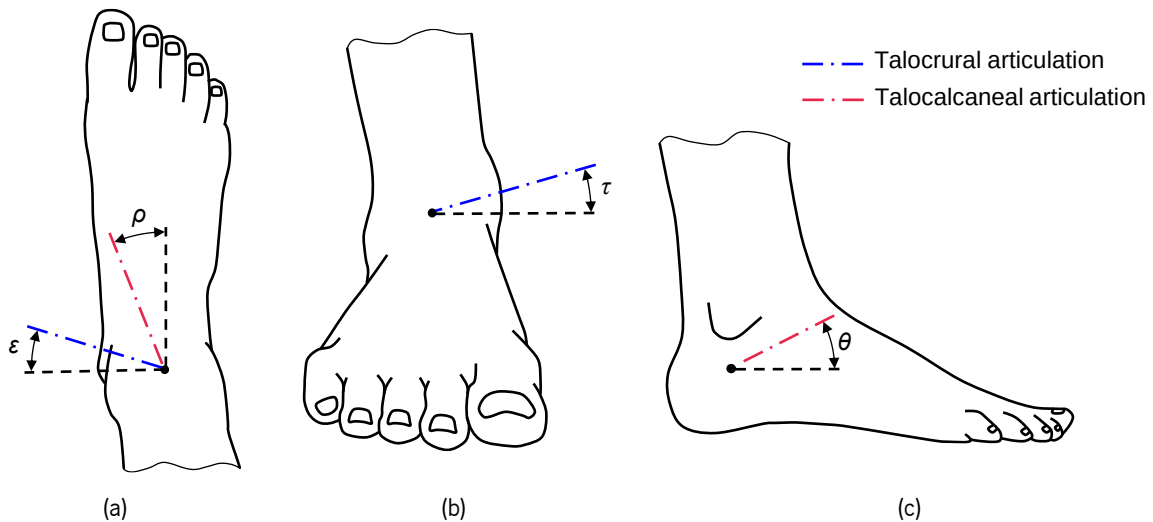


Figure 3.4 – Orientation of the talocrural and the talocalcaneal axes in the (a) transverse, (b) frontal and (c) sagittal planes.

Since the movement of a human articulation occurs around its axis, accurately modeling the second particularity of the ankle joint complex of the human foot is of utmost importance. In fact, if the axis of the articulation is incorrectly determined, the joint of the biomechanical model may allow movements that are not anatomically expected. Thus, the anatomical accuracy of the model becomes compromised, which may strongly influence the obtained results.

In general, the human foot and the ankle joint complex can be modeled in distinct manners by considering approaches with a varying degree of complexity, which mimic with more or less accuracy the

anatomical characteristics intrinsic to the foot (De Mits et al., 2012; Deschamps et al., 2011; Marta et al., 2022; Rankine et al., 2008; Roupia et al., 2022; M. Silva et al., 2021; M. R. Silva, Marques, Silva, et al., 2023). On the one hand, some models consider only the dorsiflexion and plantarflexion movements of the human foot. This is achieved by considering that the foot articulates with the leg via the talocrural articulation only, which is formulated as an ideal revolute joint, either in two- (Günther & Ruder, 2003; Peasgood et al., 2007; Shourijeh & McPhee, 2015; P. Silva et al., 2010) or three-dimensions (Burdett, 1982; Lopes et al., 2016). On the other hand, more elaborate models considering the movements allowed by both the talocrural and the talocalcaneal articulations of the human foot have also been proposed in some studies. In this sense, the ankle joint complex has been modeled either as a spherical joint (Crowninshield et al., 1978; Hardt, 1978; Kepple et al., 1997; Mouzo et al., 2018), as two (Delp et al., 1990; Dul & Johnson, 1985; Maniar et al., 2022; Razu & Guess, 2018; Reinbolt et al., 2005; S. H. Scott & Winter, 1993; van den Bogert et al., 1994) or three (Guess et al., 2014) separate revolute joints and as a classical universal joint (F. Anderson & Pandy, 1999; Y.-C. Lin & Pandy, 2017). However, modeling the ankle joint complex as a spherical or classical universal joint precludes the possibility of considering the fact that the talus separates the two articulations, preventing the talocrural and the talocalcaneal axes from intersecting. This difficulty can be addressed by using two separate revolute joints, one for each articulation, and adding the talus bone as one segment. Nevertheless, including the talus, which has a small mass and inertia, as a rigid segment on the biomechanical model not only increases the complexity of the model, but also potentially leads to numerical issues during the resolution of the equations of motion due to the calculation of high accelerations, ultimately penalizing the computational efficiency.

The available studies have not yet considered a sufficiently anatomically accurate and computationally efficient modelling of the ankle joint complex, which plays a key role in studying the movement of the human foot. Thus, a new formulation for the ankle joint complex of the human foot, which takes into consideration the two specific and crucial anatomical particularities described above, is presented. The proposed formulation has its foundations on a previously published work (Malaquias et al., 2013, 2015), and it relies on the use of a modified universal joint. The joint considers the talocrural and the talocalcaneal joints and it is incorporated with a massless link, representing the talus and mimicking the real function of this bone (see Figure 3.5a). The massless link guarantees that the distance between the two joint axes is preserved. A general representation of the proposed modified universal joint connecting bodies i and j is depicted in Figure 3.5b. The centers of mass of the bodies are O_i and O_j . Body-fixed coordinate systems $\xi\eta\zeta$ are attached to the center of mass, whilst xyz represents the global coordinate system (P. Nikravesh, 1988).

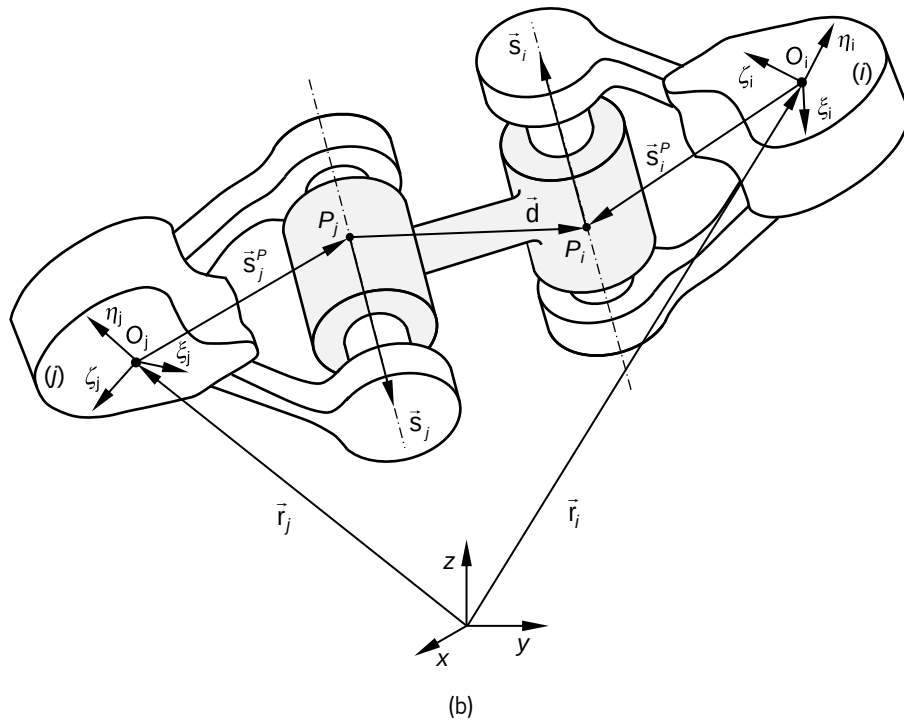
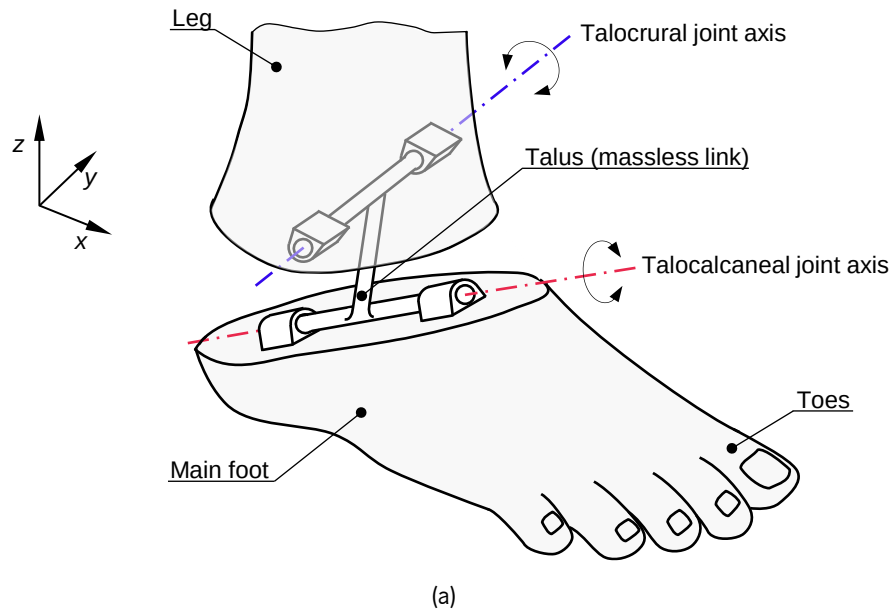


Figure 3.5 – (a) Schematic representation of the ankle joint complex of the human foot modeled as a modified universal joint. The x , y , and z directions correspond to the anteroposterior, mediolateral and superoinferior directions, respectively, in the anatomical reference position. (b) Generic configuration of a modified universal joint connecting bodies i and j .

The modified universal joint allows two relative degrees-of-freedom between the bodies i and j that are connected by the joint. Thus, four kinematic constraint equations must be considered, namely:

- (i) Establishing a constant length between points P_i and P_j on each of the joint axes (see Figure 3.5).

This constraint represents a link connecting the two bodies, which is not modeled as an actual body, but instead as a massless element (Flores, 2015; P. Nikravesh, 1988). The massless link corresponds to the talus bone of the ankle joint complex, and the constraint equation can be written as

$$\Phi_1 = \mathbf{d}^T \mathbf{d} - l_{ml}^2 = 0 \quad (3.19)$$

where l_{ml} is the length of the massless link and vector $\mathbf{d}$ is defined as (see Figure 3.5)

$$\mathbf{d} = \mathbf{r}_j^P - \mathbf{r}_i^P = \mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i - \mathbf{s}_i^P \quad (3.20)$$

in which $\mathbf{r}_k^P$ is the global position vector of point P located on body k ($k = i, j$), $\mathbf{r}_k$ denotes the position vector of the center of mass of body k described in global coordinates, and $\mathbf{s}_k^P$ is the global position vector of point P located on body k with respect to the body's local coordinate system (P. Nikravesh, 1988). The local and global components of $\mathbf{s}_k^P$ are related as

$$\mathbf{s}_k^P = \mathbf{A}_k \mathbf{s}_k'^P \quad (3.21)$$

where $\mathbf{A}_k$ ($k = i, j$) is the transformation matrix of body k and the symbol $(\prime)$ represents the components of vector $\mathbf{s}$ in the body's local coordinate system. Thus, the vector $\mathbf{s}_k'^P$ refers to the position of point P on the body's local coordinates.

(ii) Establishing a constant angle between the non-intersecting $\mathbf{s}_i$ and $\mathbf{s}_j$ joint axes vectors (see Figure 3.5). This constraint ensures that the relative orientation of vectors $\mathbf{s}_i$ and $\mathbf{s}_j$ of the modified universal joint at any given configuration is equal to the initial one, and it is formulated as

$$\Phi_2 = \mathbf{s}_i^T \mathbf{s}_j - \mathbf{s}_{i,0}^T \mathbf{s}_{j,0} = 0 \quad (3.22)$$

in which $\mathbf{s}_i$ and $\mathbf{s}_j$ represent two vectors placed on the joint axes of the modified universal joint that belong to bodies i and j , respectively, in global coordinates, and $\mathbf{s}_{i,0}$ and $\mathbf{s}_{j,0}$ are the coordinates of vectors $\mathbf{s}_i$ and $\mathbf{s}_j$ in the initial configuration, respectively.

(iii) Establishing a constant angle between vector $\mathbf{d}$ and the $\mathbf{s}_i$ joint axis vector (see Figure 3.5). This constraint is added to the formulation of the modified universal joint to maintain the relative orientation of the joint axis $\mathbf{s}_i$ and vector $\mathbf{d}$ constant in all configurations. The corresponding kinematic constraint equation can be expressed as

$$\Phi_3 = \mathbf{s}_i^T \mathbf{d} - \mathbf{s}_{i,0}^T \mathbf{d}_0 = 0 \quad (3.23)$$

where $\mathbf{d}_0$ represents the initial coordinates of vector $\mathbf{d}$.

(iv) Establishing a constant angle between vector $\mathbf{d}$ and the $\mathbf{s}_j$ joint axis vector (see Figure 3.5). The constraint equation is expressed as

$$\Phi_4 = \mathbf{s}_j^T \mathbf{d} - \mathbf{s}_{j,0}^T \mathbf{d}_0 = 0 \quad (3.24)$$

In summary, the set of kinematic constraint equations utilized to model the proposed modified universal joint can be condensed as

$$\Phi^{(u_m,4)} = \begin{cases} \mathbf{d}^T \mathbf{d} - l_{ml}^2 = 0 \\ \mathbf{s}_i^T \mathbf{s}_j - \mathbf{s}_{i,0}^T \mathbf{s}_{j,0} = 0 \\ \mathbf{s}_i^T \mathbf{d} - \mathbf{s}_{i,0}^T \mathbf{d}_0 = 0 \\ \mathbf{s}_j^T \mathbf{d} - \mathbf{s}_{j,0}^T \mathbf{d}_0 = 0 \end{cases} \quad (3.25)$$

Following the Nikravesh formulation, $\Phi^{(u_m,4)}$ refers to a modified universal joint constraint formulation containing four equations (P. Nikravesh, 1988).

The velocity constraint equations for the proposed modified universal joint are obtained by taking the first time derivative of Eq. (3.25) yielding

$$\dot{\Phi}^{(u_m,4)} = \begin{cases} 2\mathbf{d}^T (\dot{\mathbf{r}}_j + \dot{\mathbf{s}}_j^P - \dot{\mathbf{r}}_i - \dot{\mathbf{s}}_i^P) = 0 \\ \mathbf{s}_j^T \dot{\mathbf{s}}_i + \mathbf{s}_i^T \dot{\mathbf{s}}_j = 0 \\ \mathbf{d}^T \dot{\mathbf{s}}_i + \mathbf{s}_i^T (\dot{\mathbf{r}}_j + \dot{\mathbf{s}}_j^P - \dot{\mathbf{r}}_i - \dot{\mathbf{s}}_i^P) = 0 \\ \mathbf{d}^T \dot{\mathbf{s}}_j + \mathbf{s}_j^T (\dot{\mathbf{r}}_j + \dot{\mathbf{s}}_j^P - \dot{\mathbf{r}}_i - \dot{\mathbf{s}}_i^P) = 0 \end{cases} \quad (3.26)$$

The formulation of the modified universal joint relies exclusively on four kinematic constraints that are not explicit functions of time, as it can be observed in Eq. (3.25). Thus, in this particular case, vector $\mathbf{v}$, which represents the right-hand side vector of the velocity constraint equations, is null.

Equation (3.26) is not explicitly formulated in terms of the angular velocities of bodies i and j , which are essential for establishing the Jacobian matrix. In order to address this issue, a condition that relates the linear and angular velocities should be considered as (P. Nikravesh, 1988)

$$\dot{\mathbf{s}} = \tilde{\boldsymbol{\omega}} \mathbf{s} = -\tilde{\mathbf{s}} \boldsymbol{\omega} \quad (3.27)$$

where the symbol tilde ($\sim$) represents the skew symmetric matrix associated with that vector, and $\boldsymbol{\omega}$ is the angular velocity vector in global coordinates. Thus, Eq. (3.26) can be rewritten as

$$\dot{\Phi}^{(u_m,4)} = \begin{cases} 2\mathbf{d}^T (\dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \dot{\mathbf{r}}_i + \tilde{\mathbf{s}}_i^P \boldsymbol{\omega}_i) = 0 \\ -\mathbf{s}_j^T \tilde{\mathbf{s}}_i \boldsymbol{\omega}_i - \mathbf{s}_i^T \tilde{\mathbf{s}}_j \boldsymbol{\omega}_j = 0 \\ -\mathbf{d}^T \tilde{\mathbf{s}}_i \boldsymbol{\omega}_i + \mathbf{s}_i^T \dot{\mathbf{r}}_j - \mathbf{s}_i^T \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \mathbf{s}_i^T \dot{\mathbf{r}}_i + \mathbf{s}_i^T \tilde{\mathbf{s}}_i^P \boldsymbol{\omega}_i = 0 \\ -\mathbf{d}^T \tilde{\mathbf{s}}_j \boldsymbol{\omega}_j + \mathbf{s}_j^T \dot{\mathbf{r}}_j - \mathbf{s}_j^T \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \mathbf{s}_j^T \dot{\mathbf{r}}_i + \mathbf{s}_j^T \tilde{\mathbf{s}}_i^P \boldsymbol{\omega}_i = 0 \end{cases} \quad (3.28)$$

Observing Eq. (3.28), the contribution of the modified universal joint constraints to the Jacobian matrix can be established as

$$\mathbf{D}_{(4 \times 12)}^{(u_m,4)} = \begin{bmatrix} -2\mathbf{d}^T & 2\mathbf{d}^T \tilde{\mathbf{s}}_i^P & 2\mathbf{d}^T & -2\mathbf{d}^T \tilde{\mathbf{s}}_j^P \\ \mathbf{0} & -\mathbf{s}_j^T \tilde{\mathbf{s}}_i & \mathbf{0} & -\mathbf{s}_i^T \tilde{\mathbf{s}}_j \\ -\mathbf{s}_i^T & -\mathbf{d}^T \tilde{\mathbf{s}}_i + \mathbf{s}_i^T \tilde{\mathbf{s}}_i^P & \mathbf{s}_i^T & -\mathbf{s}_i^T \tilde{\mathbf{s}}_j^P \\ -\mathbf{s}_j^T & \mathbf{s}_j^T \tilde{\mathbf{s}}_i^P & \mathbf{s}_j^T & -\mathbf{d}^T \tilde{\mathbf{s}}_j - \mathbf{s}_j^T \tilde{\mathbf{s}}_j^P \end{bmatrix} \quad (3.29)$$

Finally, the time derivative of Eq. (3.26) yields the acceleration constraint equations of the modified universal joint as

$$\ddot{\Phi}^{(u_m,4)} = \begin{cases} 2\mathbf{d}^T(\ddot{\mathbf{r}}_j + \ddot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i - \ddot{\mathbf{s}}_i^P) + 2\dot{\mathbf{d}}^T\dot{\mathbf{d}} = 0 \\ \mathbf{s}_j^T\ddot{\mathbf{s}}_i + \dot{\mathbf{s}}_i^T\dot{\mathbf{s}}_j + \mathbf{s}_i^T\ddot{\mathbf{s}}_j + \dot{\mathbf{s}}_j^T\dot{\mathbf{s}}_i = 0 \\ \mathbf{d}^T\ddot{\mathbf{s}}_i + \dot{\mathbf{s}}_i^T\dot{\mathbf{d}} + \mathbf{s}_i^T(\ddot{\mathbf{r}}_j + \ddot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i - \ddot{\mathbf{s}}_i^P) + \dot{\mathbf{d}}^T\dot{\mathbf{s}}_i = 0 \\ \mathbf{d}^T\ddot{\mathbf{s}}_j + \dot{\mathbf{s}}_j^T\dot{\mathbf{d}} + \mathbf{s}_j^T(\ddot{\mathbf{r}}_j + \ddot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i - \ddot{\mathbf{s}}_i^P) + \dot{\mathbf{d}}^T\dot{\mathbf{s}}_j = 0 \end{cases} \quad (3.30)$$

Equation (3.30) is not expressed in terms of the angular accelerations of bodies i and j , which are required to establish the right-hand side vector of the acceleration equations. In order to address this issue, a condition relating the linear and angular accelerations must be utilized (P. Nikravesh, 1988)

$$\ddot{\mathbf{s}} = -\tilde{\mathbf{s}}\dot{\boldsymbol{\omega}} + \tilde{\boldsymbol{\omega}}\dot{\mathbf{s}} \quad (3.31)$$

where $\dot{\boldsymbol{\omega}}$ is the angular acceleration vector in global coordinates. Thus, Eq. (3.30) can be rewritten as

$$\ddot{\Phi}^{(u_m,4)} = \begin{cases} 2\mathbf{d}^T(\ddot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P\dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j\dot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i + \tilde{\mathbf{s}}_i^P\dot{\boldsymbol{\omega}}_i - \tilde{\boldsymbol{\omega}}_i\dot{\mathbf{s}}_i^P) + 2\dot{\mathbf{d}}^T\dot{\mathbf{d}} = 0 \\ \mathbf{s}_j^T(-\tilde{\mathbf{s}}_i\dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i\dot{\mathbf{s}}_i) + \dot{\mathbf{s}}_i^T\dot{\mathbf{s}}_j + \mathbf{s}_i^T(-\tilde{\mathbf{s}}_j\dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j\dot{\mathbf{s}}_j^P) + \dot{\mathbf{s}}_j^T\dot{\mathbf{s}}_i = 0 \\ \mathbf{d}^T(-\tilde{\mathbf{s}}_i\dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i\dot{\mathbf{s}}_i) + \dot{\mathbf{s}}_i^T\dot{\mathbf{d}} + \mathbf{s}_i^T(\ddot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P\dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j\dot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i + \tilde{\mathbf{s}}_i^P\dot{\boldsymbol{\omega}}_i - \tilde{\boldsymbol{\omega}}_i\dot{\mathbf{s}}_i^P) + \dot{\mathbf{d}}^T\dot{\mathbf{s}}_i = 0 \\ \mathbf{d}^T(-\tilde{\mathbf{s}}_j\dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j\dot{\mathbf{s}}_j^P) + \dot{\mathbf{s}}_j^T\dot{\mathbf{d}} + \mathbf{s}_j^T(\ddot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P\dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j\dot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i + \tilde{\mathbf{s}}_i^P\dot{\boldsymbol{\omega}}_i - \tilde{\boldsymbol{\omega}}_i\dot{\mathbf{s}}_i^P) + \dot{\mathbf{d}}^T\dot{\mathbf{s}}_j = 0 \end{cases} \quad (3.32)$$

Hence, observing Eq. (3.32), the contribution of the modified universal joint constraints to the right-hand side vector of the acceleration equations yields

$$\gamma^{(u_m,4)} = \begin{Bmatrix} 2\mathbf{d}^T(\tilde{\boldsymbol{\omega}}_i\dot{\mathbf{s}}_i^P - \tilde{\boldsymbol{\omega}}_j\dot{\mathbf{s}}_j^P) - 2\dot{\mathbf{d}}^T\dot{\mathbf{d}} \\ -\mathbf{s}_i^T\tilde{\boldsymbol{\omega}}_j\dot{\mathbf{s}}_j - \mathbf{s}_j^T\tilde{\boldsymbol{\omega}}_i\dot{\mathbf{s}}_i - 2\dot{\mathbf{s}}_j^T\dot{\mathbf{s}}_i \\ -\mathbf{d}^T\tilde{\boldsymbol{\omega}}_i\dot{\mathbf{s}}_i - 2\dot{\mathbf{d}}^T\dot{\mathbf{s}}_i - \mathbf{s}_i^T\tilde{\boldsymbol{\omega}}_j\dot{\mathbf{s}}_j^P + \mathbf{s}_i^T\tilde{\boldsymbol{\omega}}_i\dot{\mathbf{s}}_i^P \\ -\mathbf{d}^T\tilde{\boldsymbol{\omega}}_j\dot{\mathbf{s}}_j - 2\dot{\mathbf{d}}^T\dot{\mathbf{s}}_j - \mathbf{s}_j^T\tilde{\boldsymbol{\omega}}_i\dot{\mathbf{s}}_i^P - \mathbf{s}_j^T\tilde{\boldsymbol{\omega}}_j\dot{\mathbf{s}}_j^P \end{Bmatrix} \quad (3.33)$$

In comparison with the currently-existing ankle models, the use of the proposed massless link approach has several advantages: (i) the physiological distance between the talocrural and the talocalcaneal articulations is preserved; (ii) the specific anatomical orientations of the joint axes are considered, (iii) the impossibility of measuring the talus motion using non-invasive techniques is avoided, (iv) the overall complexity of the biomechanical model is not increased as the number of coordinates and constraints is kept unchanged; (v) the addition of a segment with very small mass and inertia in the mass matrix is avoided. This last issue is of paramount importance since a segment with small mass and inertia would result in the calculation of significantly high accelerations during the resolution of the equations of motion (3.14). The calculation of such high values for the accelerations would ultimately decrease the integration time of the system and lower its computational efficiency. Concerning advantage (iii), since the talus is an internal bone that is hidden by the surrounding tibia, fibula and calcaneus bones, its motion is impossible to measure when acquiring experimental data with non-invasive techniques, such as the use of skin markers (Sancisi & Parenti-Castelli, 2013; van den Bogert et al., 1994). The use of the massless link approach overcomes this difficulty, eliminating the need for experimental measurement of talus motion.

3.3. Methodology to Restrict the Range of Motion of Joints

In a simple manner, the range of motion (RoM) can be defined as the relative amplitude of motion permitted at a joint and it is influenced by the geometric configuration of the bodies adjacent to the joint, by the joint itself, and by the materials existing around the joint. The materials allow energy dissipation and have an effect on the functionality and durability of the joint. In the multibody systems methodology, mechanical joints are typically formulated as classical kinematic constraints, which do not allow the restriction of the RoM of the bodies connected by them. In other words, the RoM is limitless and unrestricted. These features are not compatible with actual mechanical joints, where some bounds are necessary from the functional and operating point of view. Thus, additional restrictions to prevent the joints from performing movements that are not acceptable and to avoid unrealistic or unacceptable configurations of the connected bodies must be incorporated into the formulation. Although this may not be a problem for some studies, in many applications, the mechanical joints are subjected to physical limits. Consequently, the restriction of the RoM of the bodies connected by mechanical joints is required to allow the appropriate functioning of the multibody system. Two typical examples where the restriction to the RoM on the joints is utilized are in car suspensions (Ambrósio & Pombo, 2018; Lv et al., 2021) and in human articulations (Duprey et al., 2017; Quental et al., 2012; Ribeiro et al., 2012; Sancisi et al., 2017), in which the relative motion associated with them is restricted by the physical limits related to the adjacent bodies and actual joint nature. Hence, the development of methodologies that realistically and accurately restrict the RoM of mechanical joints is needed to correctly model multibody systems, providing accurate results.

There are several methods in the literature that allow the restriction of the RoM of joints (F. Anderson & Pandy, 1999; Audu & Davy, 1985; Davy & Audu, 1987; Hatze, 1976; Nagano et al., 2005, 2007; Yamaguchi, 2001). However, the approach proposed by M. P. T. Silva et al. (1997), which applies a penalty moment when the RoM is exceeded, is the foundation for the methodology proposed in this section. The proposed methodology extends and improves the approach presented by M. P. T. Silva et al. (1997), specifically in what regards to the definition of the RoM limits, the calculation of the penalty moments and the establishment of their direction of application. Hence, the preservation of the mechanical energy of the system is guaranteed when an elastic resistance is considered. The RoM limits are defined based on a circumduction cone, which makes this methodology specifically targeted to joints allowing rotational degrees-of-freedom, namely spherical, revolute, or universal joints. The proposed methodology is best suitable to be applied in forward multibody dynamic simulations, guaranteeing that the joints do not reach unfeasible positions.

Joint resistance moments are applied to the connected bodies to mimic the dissipative behavior of the materials constituent of mechanical joints and to prevent unacceptable configurations of those bodies. Thus, two terms contribute to the calculation of the joint resistance moments, $\mathbf{m}_h^r$, as

$$\mathbf{m}_h^r = \mathbf{m}_h^d + \mathbf{m}_h^{\text{mr}} \quad (3.34)$$

where $\mathbf{m}_h^d$ is the dissipative moment vector, and $\mathbf{m}_h^{\text{mr}}$ represents the motion-restricting moment vector. The subscript h denotes the joint index.

With the purpose to better understand the proposed methodology, it is of paramount importance to become familiar with the concepts of reference body and moving body. Any type of mechanical joint connects two bodies, and it is assumed that one of those bodies is named the reference body and the other is the moving body. While the moving body is the one which RoM is intended to be restricted, the reference body enables the definition of the limits inside which the moving body can freely move without exceeding the RoM of the joint. A schematic representation of a multibody mechanical system composed of two bodies i and j , which are the reference and moving bodies, respectively, connected by a spherical joint h is presented in Figure 3.6.

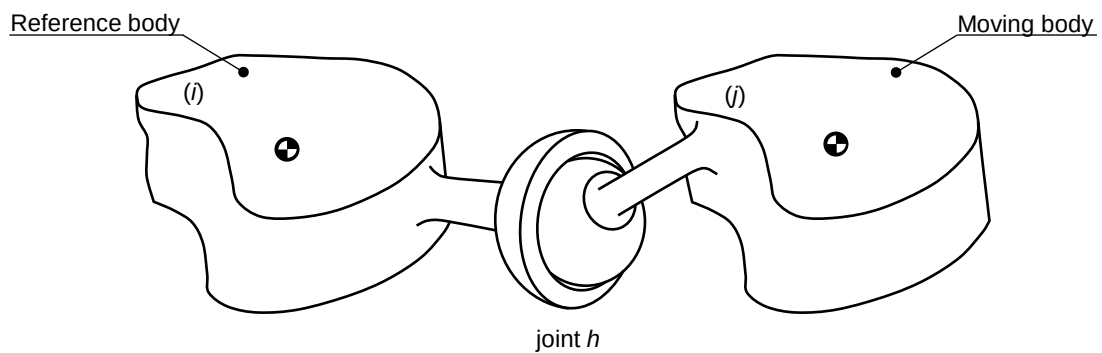


Figure 3.6 – Schematic representation of a multibody mechanical system composed of bodies i and j , which represent the reference and moving bodies, respectively, connected by a spherical joint h .

The proposed methodology is described for a spherical joint since it represents the most general case. However, it can be applied to any type of mechanical joint with rotational degrees-of-freedom, including, for instance, revolute, cylindrical, or universal joints.

3.3.1. Joint Motion-Restricting Moment

The joint motion-restricting moment acts to restrict the RoM of the mechanical joint, and it is typically modeled as an element with a non-linear elastic behavior. The joint motion-restricting moment is null during admissible joint motions, i.e., within the allowable RoM for that specific joint, and varies

from zero to a maximum value whenever an unacceptable configuration of the moving body is detected. It should be noticed that the transition from null to the maximum moment magnitude occurs in a very short angular range (M. P. T. Silva et al., 1997). In the following paragraphs, the ingredients for the calculation of the joint motion-restricting moment are described in detail.

Circumduction Cone Definition

The definition of the circumduction cone for the considered mechanical joint is the first step to calculate the joint motion-restricting moment. Circumduction combines the movements about the three geometric planes of the Cartesian coordinate system, and when it is taken to its maximum latitude, the moving body describes a cone in space, which is the cone of circumduction. The circumduction cone is defined as the three-dimensional surface inside which any configuration of the joint is possible. Thus, the RoM of the joints is associated with the working space of the circumduction cone. The apex of the cone is considered to be located at the center of the joint (Kapandji, 1974; M. P. T. Silva et al., 1997), as it can be observed in Figure 3.7. The circumduction cone can be established for any joint with rotational degrees-of-freedom, independently of its number of degrees-of-freedom. In the particular case of a revolute joint, some sections of the circumduction cone are not reached by the moving body due to the intrinsic kinematic structure of this type of joint. If a mechanical joint allows simultaneous rotation around more than one joint axis and the axes intersect at a specific point, as in the case of spherical and classical universal joints, the RoM of that mechanical joint can be restricted by only one circumduction cone. In turn, if composite joints (Flores, 2015; P. Nikravesh, 1988) are considered, such as modified universal or spherical-spherical joints, the RoM associated with each joint axis must be restricted using different circumduction cones. The internal rotational degree-of-freedom is not restricted by this methodology.

The circumduction cone is characterized by defining the axes of the joint's local coordinate system using the local coordinate system of the reference body (body i), which can be defined arbitrarily. The joint's and reference body's local coordinate systems may not necessarily be coincident. The joint's local coordinate system must be defined in the most convenient manner, depending on the specificities of the multibody system under analysis. In the cone illustrated in Figure 3.7, the unit vectors defining the axes $\mathbf{u}'_{\xi,h}$ and $\mathbf{u}'_{\eta,h}$ of the joint's local coordinate system are defined as

$$\mathbf{u}'_{\xi,h} = \{0 \quad 0 \quad -1\}^T \quad \text{and} \quad \mathbf{u}'_{\eta,h} = \{0 \quad 1 \quad 0\}^T$$

The local and global components of a vector $\mathbf{u}$ relate using an expression similar to Eq. (3.21).

The $\mathbf{u}_{\zeta,h}$ unit vector of the joint's local coordinate system is obtained by the cross product of the $\mathbf{u}_{\xi,h}$ and $\mathbf{u}_{\eta,h}$ unit vectors as

$$\mathbf{u}_{\zeta,h} = \tilde{\mathbf{u}}_{\xi,h} \mathbf{u}_{\eta,h} \quad (3.35)$$

After the definition of the joint's local coordinate system, a unit vector, $\mathbf{u}_{r,h}$, must be established using the moving body's (body j) local coordinate system. This vector allows to identify, at every configuration, the orientation of the moving body in the joint's local coordinate system. Analyzing the cone illustrated in Figure 3.7, vector $\mathbf{u}'_{r,h}$ is defined as

$$\mathbf{u}'_{r,h} = \{1 \ 0 \ 0\}^T$$

The unit vector $\mathbf{u}_{r,h}$ should not be defined such that its initial configuration is outside the circumduction cone, thus, being in an unacceptable configuration. Although it is not mandatory, the unit vector and the joint's local coordinate system are defined such that the vector $\mathbf{u}_{r,h}$ and the local ζ_h axis of the joint's local coordinate system are coincident at the initial configuration, as observed in Figure 3.7.

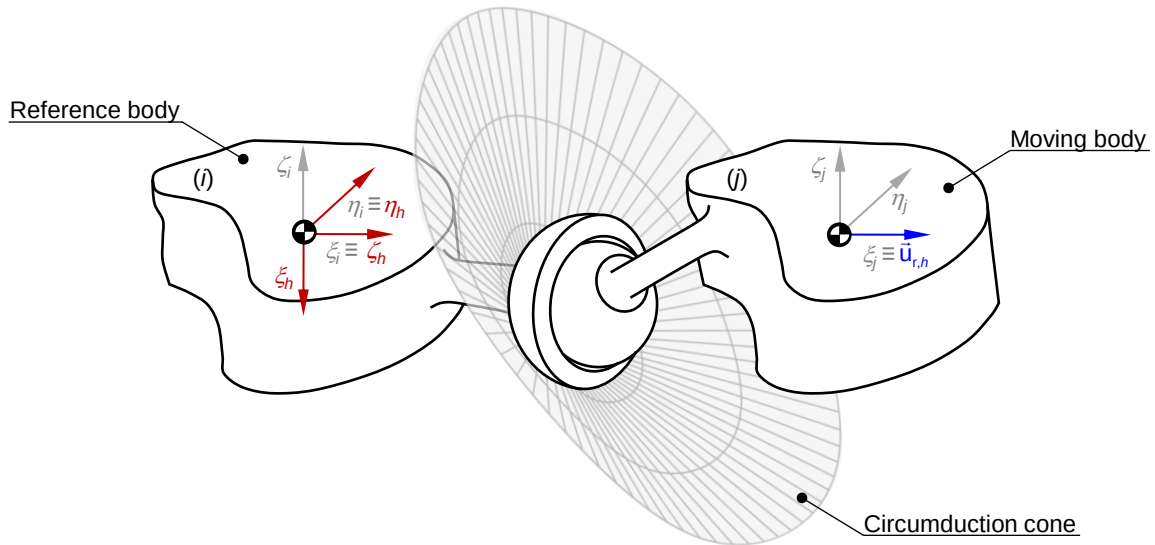


Figure 3.7 – Schematic representation of a system composed of bodies i and j , which represent, respectively, the reference and moving bodies, connected by a general rotational mechanical joint h . The circumduction cone, the joint's local reference ξ_h, η_h, ζ_h and the unit vector $\mathbf{u}_{r,h}$ are represented.

The moving body is considered to be in an acceptable configuration whenever it is located inside the circumduction cone, as it is depicted in Figure 3.7. On the contrary, if the moving body is located outside the circumduction cone, as it can be observed in Figure 3.8, it is considered to be in an unacceptable configuration. In this situation, a joint motion-restricting moment must be applied to reposition the moving body into an acceptable configuration.

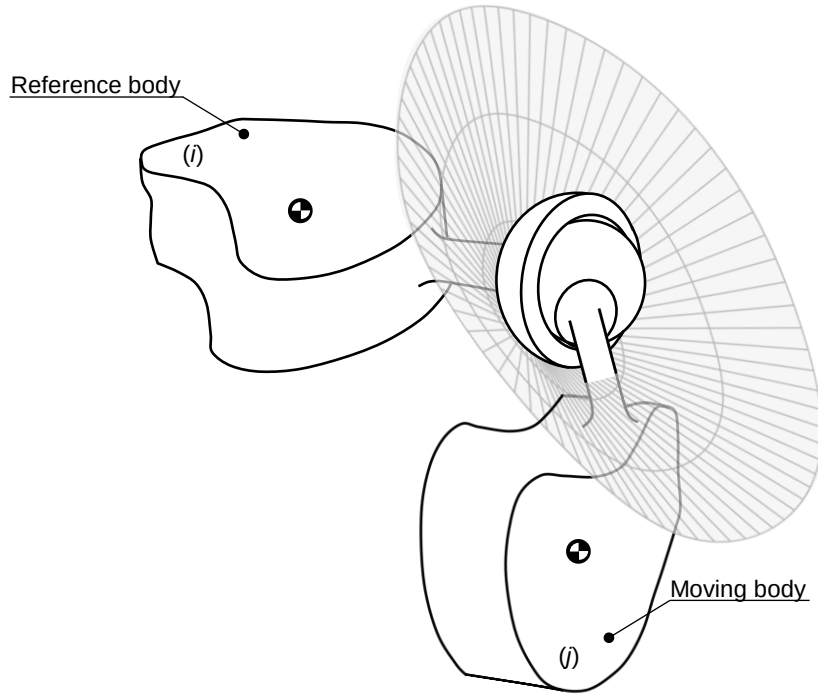


Figure 3.8 – Schematic representation of the moving body in an unacceptable configuration.

In order to determine whether the actual position of the moving body is inside (acceptable configuration) or outside (unacceptable configuration) the circumduction cone, the longitude, ψ_h , and latitude, σ_h , of the unit vector $\mathbf{u}_{r,h}$ expressed in the joint's local coordinate system must be determined.

The local and global components of a vector $\mathbf{u}$ in the joint's local coordinate system relate as

$$\mathbf{u} = \mathbf{A}_i \mathbf{B}_h \mathbf{u}'' \quad (3.36)$$

where $\mathbf{B}_h$ is the transformation matrix of joint h , and the symbol $(\prime\prime)$ represents the components of vector $\mathbf{u}$ in the joint's local coordinate system.

The longitude, ψ_h , is established by the joint's local ξ_h axis and the projection of vector $\mathbf{u}_{r,h}''$ in the plane $\xi_h \eta_h$ of the joint's local coordinate system (see Figure 3.9a). Therefore, ψ_h is calculated as

$$\psi_h = \arctan \left(\frac{u_{r,h,\eta}''}{u_{r,h,\xi}''} \right) \quad (3.37)$$

It is important to note that, in Eq. (3.37), the atan2 function, which denotes the four-quadrant inverse tangent, must be utilized. The atan2 function returns values in the closed interval $[-\pi, \pi]$, and, therefore, whenever ψ_h calculated using Eq. (3.37) is negative, a value of 2π must be added to ψ_h in order to obtain values in the closed interval $[0, 2\pi]$.

The latitude, σ_h , is established by the joint's local unit vector $\mathbf{u}_{\zeta,h}$ and the unit vector $\mathbf{u}_{r,h}$, both expressed in the joint's local coordinate system (see Figure 3.9b). The latitude can be calculated as

$$\sigma_h = \arccos(\mathbf{u}_{r,h}''^T \mathbf{u}_{\zeta,h}'') \quad (3.38)$$

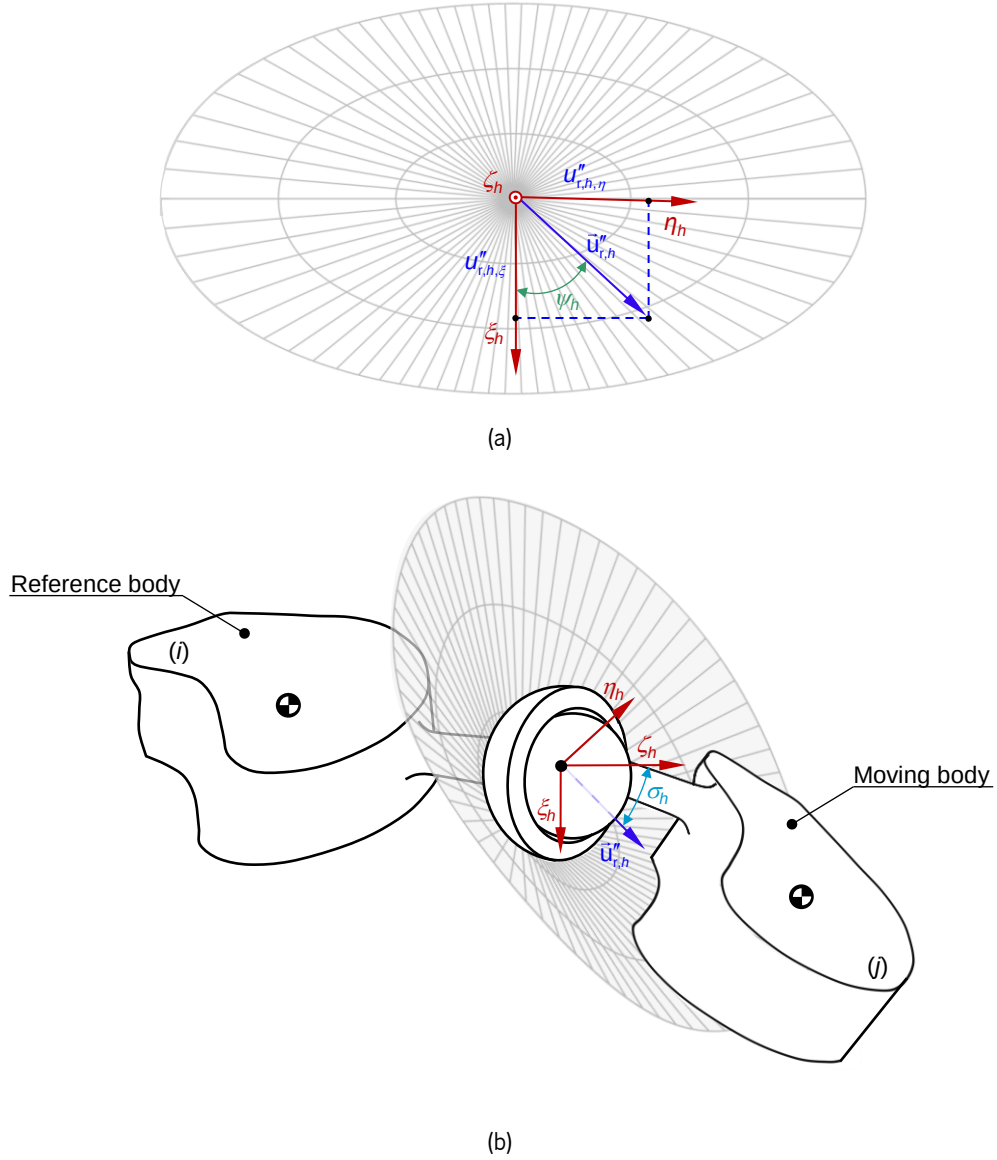


Figure 3.9 – Schematic representation of the (a) longitude, ψ_h , and (b) latitude, σ_h , utilized in the calculation of the joint motion-restricting moment. The longitude is defined in the plane $\xi_h \eta_h$ of the joint's local coordinate system (top view of the circumduction cone).

At this stage, it must be noticed that all the necessary ingredients to construct the circumduction cone have been described. The cone is defined by specifying the maximum allowable latitude, $\sigma_{h,\max}$, for certain values of longitude, ψ_h . The longitude and latitude must be defined in the closed interval $[0, 2\pi]$ and $[0, \pi]$ radians, respectively. Indeed, the longitude must cover all the entire domain between zero and 2π , meaning that the first and last values of longitude must always be zero and 2π . On the other hand, the maximum latitude can assume any value in the interval $[0, \pi]$ radians. For the sake of simplicity, the examples given in this section are in degrees. The simplest circumduction cone can be constructed

such that, for all values of longitude, the maximum allowable latitude has always the same value, as it can be observed in Figure 3.10a. In this case, the cone is considered regular, and it may be defined as

$$\psi_h = \{0^\circ \quad 90^\circ \quad 180^\circ \quad 270^\circ \quad 360^\circ\} \quad \text{and} \quad \sigma_{h,\max} = \{30^\circ \quad 30^\circ \quad 30^\circ \quad 30^\circ \quad 30^\circ\}$$

The level of complexity of the circumduction cone increases by specifying different values of maximum allowable latitude for the values of longitude, thus defining an irregular cone, as it can be seen in Figure 3.10b. The longitude is defined as in the above expression and the latitude can be specified as

$$\sigma_{h,\max} = \{60^\circ \quad 30^\circ \quad 45^\circ \quad 20^\circ \quad 60^\circ\}$$

It must be highlighted that the maximum allowable latitude must have the same value for 0 and 2π radians of longitude, otherwise, the circumduction cone would present a discontinuity.

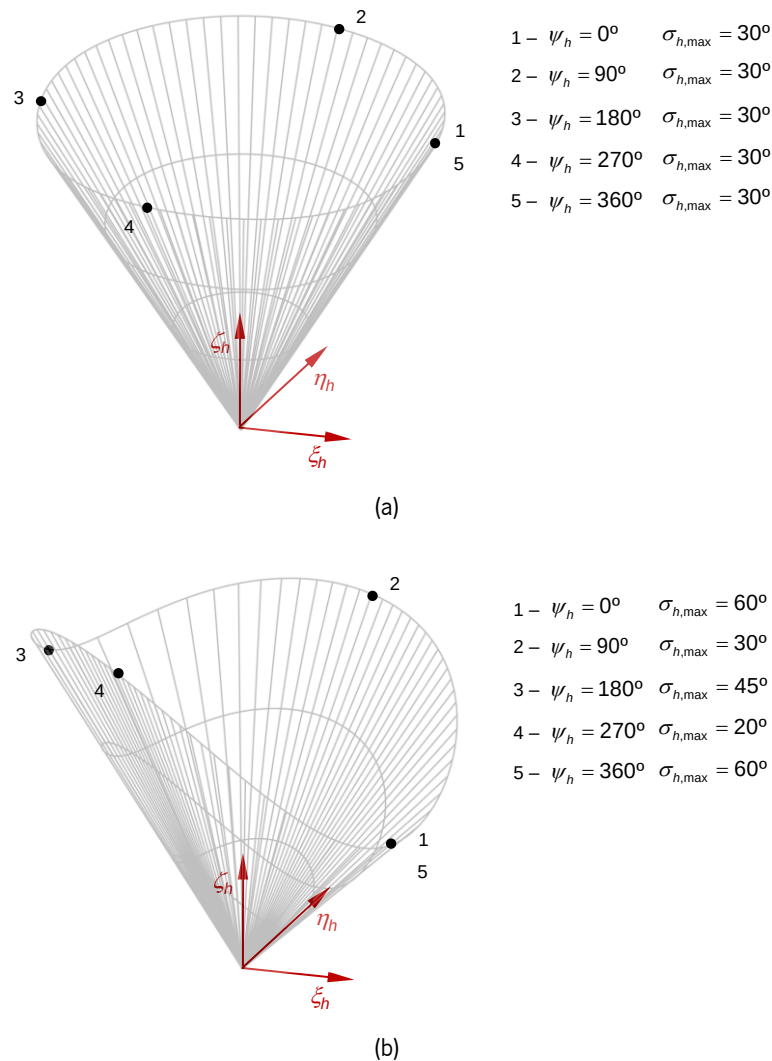


Figure 3.10 – Examples of (a) a regular and (b) an irregular circumduction cone.

The definition of the longitude and maximum latitude is dependent on several factors, including (i) the kinematic structure of the joint itself, that is, whether it is a spherical, revolute, universal, or

cylindrical joint; (ii) the definition of the local coordinate system of the joint; and (iii) the topology of the bodies of the system under analysis.

The examples presented above are utilized to simply illustrate the definition of the circumduction cone. The longitude can be defined in any arbitrary location, and the latitude essentially establishes the aperture of the circumduction cone. This cone can be defined in multiple manners, depending on the type of joint considered, its RoM, and the multibody system under analysis.

Based on the values of longitude and maximum allowable latitude utilized to define the circumduction cone, an interpolation curve is utilized to determine the values of maximum allowable latitude corresponding to any value of longitude. When the longitude is defined as in the above example, i.e., with 90° intervals, an elliptical approach is considered for the interpolation. Otherwise, a polynomial approach is employed. This topic is addressed in the following sections. At every configuration of the multibody system, both the latitude, longitude, and the corresponding maximum allowable latitude are calculated to assess whether or not the moving body is located in an unacceptable configuration, and, thus, exceeding or not the RoM of the joint.

General Problem Description

Figure 3.11 shows the top view of an irregular circumduction cone. In a specific configuration of the multibody system, the unit vector $\mathbf{u}_{r,h}''$ is pointing at A . Point B represents the point located at the surface of the circumduction cone closest to point A , since it fulfills the minimum distance condition, i.e., for those values of longitude $\psi_{h,A}$ and latitude $\sigma_{h,A}$ corresponding to point A , a vector tangent to the cone's surface, $\mathbf{t}''$, is perpendicular to the vector $\mathbf{d}_{AB}''$ connecting points A and B . Thus, B is the point of interest to calculate the maximum allowable latitude at that configuration.

In order to detect whether the joint's RoM is exceeded, i.e., to determine if the actual position of the moving body is inside or outside the circumduction cone, the latitude, $\sigma_{h,A}$, longitude, $\psi_{h,A}$, and the corresponding maximum allowable latitude, $\sigma_{h,max,A}$, at point A must be calculated. The longitude and latitude are calculated using Eqs. (3.37) and (3.38), respectively. The maximum latitude is calculated using either the elliptical or polynomial approaches described in the following paragraphs. If, for a certain longitude, $\psi_{h,A}$, the moving body is inside the circumduction cone (acceptable configuration), i.e., $\sigma_{h,A} < \sigma_{h,max,A}$, no joint motion-restricting moment is applied. However, if the moving body is outside the circumduction cone (unacceptable configuration), i.e., $\sigma_{h,A} > \sigma_{h,max,A}$, as it is displayed in Figure 3.11, the joint motion-restricting moment must be applied to the connected bodies. In these circumstances,

the longitude at point B , $\psi_{h,B}$, and the corresponding maximum allowable latitude, $\sigma_{h,\max,B}$, must be calculated to allow the correct estimation of the joint motion-restricting moment. In Figure 3.11, the difference between $\sigma_{h,\max,A}$ and $\sigma_{h,\max,B}$, and $\psi_{h,A}$ and $\psi_{h,B}$ is exaggerated for visualization purposes only. In reality, these values are very close, and, in the case of a regular cone, they are even coincident.

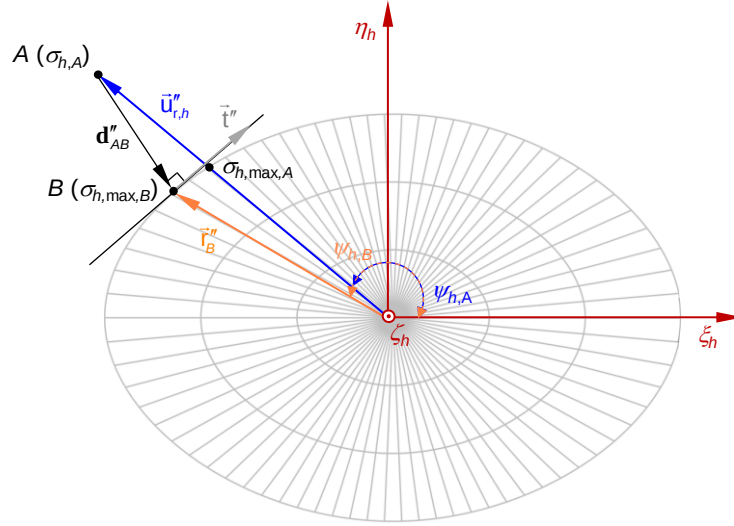


Figure 3.11 – Schematic representation of the top view of an irregular circumduction cone.

Calculation of the Maximum Allowable Latitude

In order to calculate the maximum allowable latitude, $\sigma_{h,\max}$, at points A and B , either the elliptical or the polynomial approaches must be considered. In the following paragraphs, a detailed explanation of both approaches is given using a generic point C .

The elliptical approach uses the ellipse equation, which is expressed as (see Figure 3.12)

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \quad (3.39)$$

where x and y are the Cartesian coordinates of a certain point C located on the ellipse, and a and b are constants representing the length of the semi-axes of the ellipse.

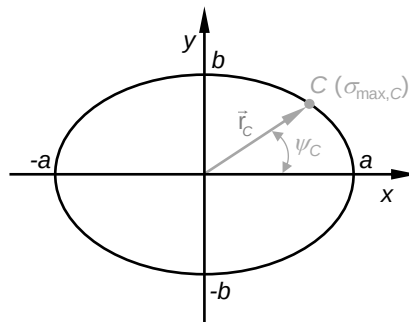


Figure 3.12 – Schematic representation of an ellipse with a certain point C described using the longitude and the latitude.

Observing Figure 3.12, the values of longitude and maximum latitude can be obtained as

$$\psi_h = \arctan\left(\frac{y}{x}\right) \quad (3.40)$$

$$\sigma_{h,\max} = \|\mathbf{r}_C\| = \sqrt{x^2 + y^2} \quad (3.41)$$

where the symbol ($\|\cdot\|$) represents the norm of vector $\mathbf{r}_C$. Similarly to Eq. (3.37), the atan2 function must be utilized in Eq. (3.40).

The ellipse equation (3.39) can be rewritten in terms of the y coordinate of point C as

$$y = \pm b \sqrt{1 - \frac{x^2}{a^2}} \quad (3.42)$$

Then, Eq. (3.42) can be substituted into Eq. (3.40) to obtain the corresponding x coordinate as

$$x = \pm \sqrt{\frac{b^2 a^2}{a^2 \tan^2(\psi_h) + b^2}} \quad (3.43)$$

Finally, substituting Eqs. (3.42) and (3.43) into Eq. (3.41), it is possible to obtain the expression for $\sigma_{h,\max}$ as a function of ψ_h using the elliptical approach as

$$\sigma_{h,\max}(\psi_h) = \sqrt{\frac{b^2}{\tan^2(\psi_h) + \frac{b^2}{a^2}} \left(1 - \frac{b^2}{a^2}\right) + b^2} \quad (3.44)$$

In the elliptical approach of the proposed RoM methodology, the values of the ellipse semi-axes, illustrated in Figure 3.12, correspond to the maximum allowable latitude for five specific values of longitude, namely 0° , 90° , 180° , 270° and 360° . These longitude values allow to divide the ellipse into four sections, which correspond to the four quadrants. Based on the value of current longitude calculated using Eq. (3.37), it is possible to determine in which quadrant of the ellipse the moving body is located. Hence, it is only necessary to evaluate the maximum allowable latitude that delimit the quadrant, which corresponds to the values of a and b . In the elliptical approach, the top view of the circumduction cone can be similar to Figure 3.13, in which four different quarters of ellipses are present on each of the four quadrants, each quarter having different values for maximum allowable latitude. Since, at each configuration, only the quarters of ellipse are considered, it is not mandatory to strictly consider circumduction cones with the shape illustrated in Figure 3.12.

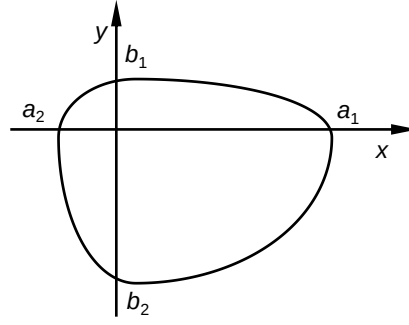


Figure 3.13 – Schematic representation of the top view of a certain circumduction cone partitioned into quarters of ellipses.

After knowing the current longitude and, consequently, on which quarter of the ellipse the moving body is located, the following condition can be applied to determine the corresponding values of a and b to utilize in Eq. (3.44) (see Figure 3.13)

$$\begin{cases} a = a_1, b = b_1 & \text{if } 0^\circ \leq \psi_h < 90^\circ \\ a = a_2, b = b_1 & \text{if } 90^\circ \leq \psi_h < 180^\circ \\ a = a_2, b = b_2 & \text{if } 180^\circ \leq \psi_h < 270^\circ \\ a = a_1, b = b_2 & \text{if } 270^\circ \leq \psi_h \leq 360^\circ \end{cases} \quad (3.45)$$

Due to the inherent characteristics of the ellipse equation, Eq. (3.39), a limitation of the elliptical approach is that it only allows to define circumduction cones in which the maximum allowable latitude is known for five specific longitude, namely 0° , 90° , 180° , 270° and 360° . However, depending on the particularities of the joint to be modeled, maximum latitude values for other values of longitude may need to be defined. Thus, in a more general approach, the polynomial approach must be considered.

A general expression for a polynomial of degree n can be written in the form

$$f(l) = \sum_{q=0}^n c_q l^q \quad (3.46)$$

where c represents the coefficients of the polynomial, k allows to identify the polynomial curve and l defines the length of the line that is zero when $\psi_h = 0^\circ$ and it is equal to the perimeter of the base of the circumduction cone (top view) when $\psi_h = 360^\circ$, as it can be observed in Figure 3.14.

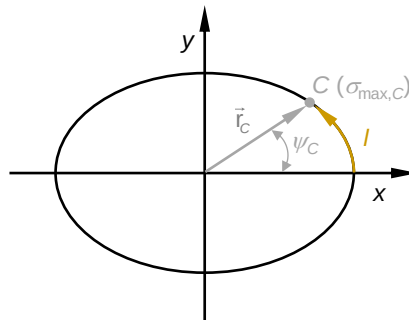


Figure 3.14 – Schematic representation of the variable l utilized in the polynomial approach.

Adopting a periodic cubic spline curve ($n=3$) to interpolate the longitude and maximum latitude values, the number of polynomial curves that compose the periodic spline is dependent on the number of ψ_h and $\sigma_{h,\max}$ values utilized to define the circumduction cone. For instance, consider an irregular circumduction cone characterized by the following longitude and maximum latitude

$$\Psi_h = \{0^\circ \quad 45^\circ \quad 180^\circ \quad 225^\circ \quad 360^\circ\} \quad \text{and} \quad \sigma_{h,\max} = \{45^\circ \quad 30^\circ \quad 45^\circ \quad 30^\circ \quad 45^\circ\}$$

Five values are utilized for the longitude and maximum latitude, therefore, four polynomial curves ($k=1, 2, 3, 4$) must be considered for the periodic spline. The spline must be periodic because the function to interpolate, which contains the longitude and maximum latitude characteristic of the joint, repeats in the interval between the first and the last defined points. Figure 3.15 depicts a schematic representation of this particular situation, where the different polynomial curves are highlighted in distinct shades of blue.

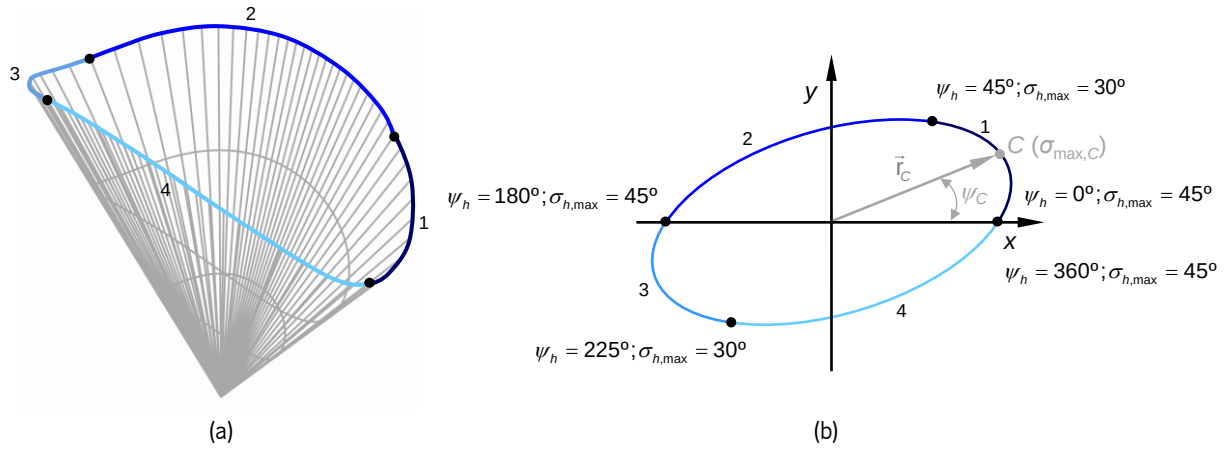


Figure 3.15 – Schematic representation of a circumduction cone with four polynomial curves highlighted in distinct shades of blue. (a) Perspective and (b) top views. The polynomial curve numbers are displayed in the figure.

Similarly to the elliptical approach, in the polynomial approach, $\sigma_{h,\max}(\psi_h)$ can be determined using Eq. (3.41). However, in this case, the x and y coordinates of a certain point C (see Figure 3.15b) are described by a cubic spline curve and given by the following conditions

$$x = c_{x,3}^k l^3 + c_{x,2}^k l^2 + c_{x,1}^k l + c_{x,0}^k \quad (3.47)$$

$$y = c_{y,3}^k l^3 + c_{y,2}^k l^2 + c_{y,1}^k l + c_{y,0}^k \quad (3.48)$$

Since point C in Figure 3.15b is located between longitude values of 0° and 45° , the first polynomial curve (darkest blue curve) must be utilized, and, thus, $k=1$.

It is possible to observe that, substituting Eqs. (3.47) and (3.48) into Eq. (3.41), the maximum allowable latitude is not explicitly dependent on the longitude, as it is in Eq. (3.44) of the elliptical approach. For the polynomial approach, the expression for $\sigma_{h,\max}$ is as

$$\sigma_{h,\max} = \sqrt{\left(c_{x,3}^k l^3 + c_{x,2}^k l^2 + c_{x,1}^k l + c_{x,0}^k\right)^2 + \left(c_{y,3}^k l^3 + c_{y,2}^k l^2 + c_{y,1}^k l + c_{y,0}^k\right)^2} \quad (3.49)$$

In this situation, the variable l must be calculated by solving a set of nonlinear equations using an iterative method, such as the Newton-Raphson method, and considering the following condition

$$\psi_h = \arctan \left(\frac{c_{y,3}^k l^3 + c_{y,2}^k l^2 + c_{y,1}^k l + c_{y,0}^k}{c_{x,3}^k l^3 + c_{x,2}^k l^2 + c_{x,1}^k l + c_{x,0}^k} \right) \quad (3.50)$$

After calculating the variable l using Eq. (3.50), the maximum allowable latitude corresponding to the longitude for the polynomial approach can be calculated using Eq. (3.49).

In a similar manner to the elliptical approach, it is possible to determine where the moving body is located based on the value of current longitude calculated using Eq. (3.37). In this case, the calculus is utilized to evaluate the corresponding polynomial curve to use ($k=1, 2, 3$ or 4 , in the example of Figure 3.15), which allows to determine the maximum allowable latitude. For example, consider that $\psi_C = 22.50^\circ$, as it can be observed in Figure 3.15b. In this situation, it is clear the moving body is located between longitude values of 0° and 45° , and the polynomial curve to use is the darkest blue one ($k=1$). The corresponding coefficients of that polynomial curve are utilized to solve the nonlinear Eqs. (3.47) and (3.48), which allow to ultimately calculate $\sigma_{h,\max}$ using Eq. (3.49).

Calculation of the Longitude: Parametrization of the Circumduction Cone

In the previous paragraphs, it was concluded that five quantities must be determined in this methodology, namely the longitude at points A and B , latitude at point A , and maximum allowable latitude at points A and B . In order to detect whether the RoM is exceeded, the longitude, latitude, and maximum allowable latitude at point A are determined using Eqs. (3.37), (3.38) and (3.44) or (3.49), respectively. If the RoM is exceeded, i.e., $\sigma_{h,A} > \sigma_{h,\max,A}$, the joint motion-restricting moment must be correctly estimated and applied to the bodies connected by the mechanical joint h . In these circumstances, the longitude at point B must be calculated. In the following paragraphs, a parametrization of the circumduction cone is considered as the method for the calculation of $\psi_{h,B}$.

The magnitude and direction of the joint motion-restricting moment is dependent on the geometry of the circumduction cone, i.e., whether it is regular or irregular, as described above (see Figure 3.10). Therefore, a parametrization procedure is implemented on the circumduction cone, which means that any point B on the cone's surface can be defined by two parameters, namely the distance to the apex, G , and the longitude, ψ_h . In the following paragraphs, a detailed explanation of this procedure is presented.

For a specific configuration, the moving body is characterized by a longitude ψ_h and a latitude σ_h . Let consider a vector with length G defined in the joint's local coordinate system as

$$\mathbf{v}_r'' = \{0 \quad 0 \quad G\}^T \quad (3.51)$$

In order to determine the coordinates of a certain position vector $\mathbf{r}''$, vector $\mathbf{v}_r''$ must be rotated, initially, σ_h around the η_h axis of the joint's local coordinate system, and then rotated ψ_h around the ζ_h axis of the same coordinate system. These rotations are mathematically described by the following conditions

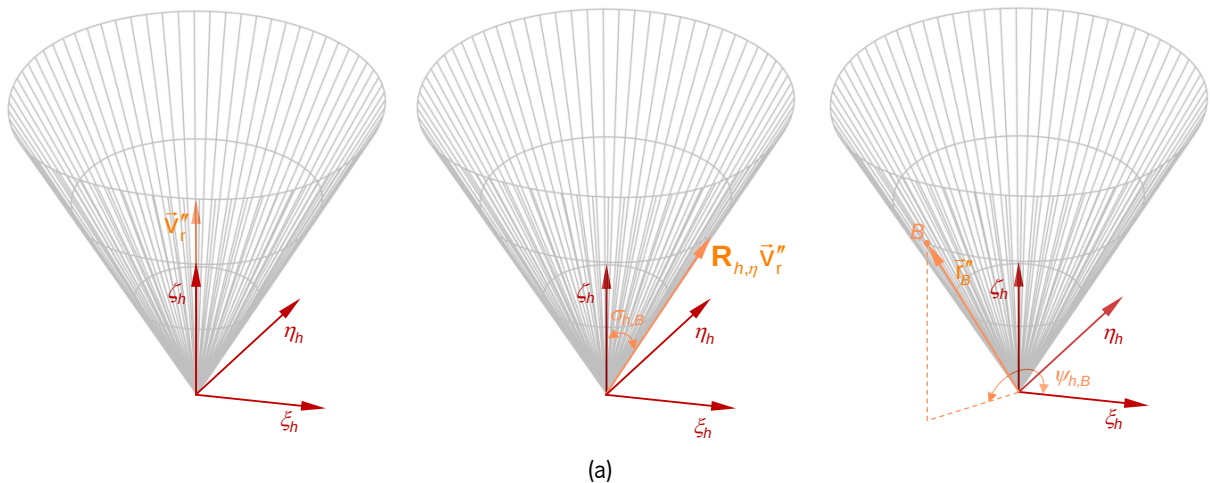
$$\begin{aligned} \mathbf{r}'' &= \mathbf{R}_{h,\zeta} \mathbf{R}_{h,\eta} \mathbf{v}_r'' \\ &= \begin{bmatrix} \cos(\psi_h) & -\sin(\psi_h) & 0 \\ \sin(\psi_h) & \cos(\psi_h) & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos(\sigma_h) & 0 & \sin(\sigma_h) \\ 0 & 1 & 0 \\ -\sin(\sigma_h) & 0 & \cos(\sigma_h) \end{bmatrix} \begin{Bmatrix} 0 \\ 0 \\ G \end{Bmatrix} \\ &= \begin{Bmatrix} G \cos(\psi_h) \sin(\sigma_h) \\ G \sin(\psi_h) \sin(\sigma_h) \\ G \cos(\sigma_h) \end{Bmatrix} \end{aligned} \quad (3.52)$$

where $\mathbf{R}_{h,\zeta}$ and $\mathbf{R}_{h,\eta}$ are transformation matrices that produce rotations about the joint's local ζ_h and η_h axes, respectively.

If the position vector $\mathbf{r}''$ is assumed to be located at the surface of the circumduction cone, $\mathbf{r}_B''$, the latitude establishes the maximum allowable latitude, which is expressed as a function of the longitude, i.e., $\sigma_{h,\max,B}(\psi_{h,B})$. In this sense, vector $\mathbf{r}_B''$ is written as

$$\mathbf{r}_B'' = \begin{Bmatrix} G \cos(\psi_{h,B}) \sin(\sigma_{h,\max,B}(\psi_{h,B})) \\ G \sin(\psi_{h,B}) \sin(\sigma_{h,\max,B}(\psi_{h,B})) \\ G \cos(\sigma_{h,\max,B}(\psi_{h,B})) \end{Bmatrix} \quad (3.53)$$

in which $\sigma_{h,\max,B}(\psi_{h,B})$ is calculated using either Eq. (3.44) or (3.49), depending on whether the elliptical or polynomial approaches are considered, respectively. The rotations explained in the previous paragraphs are illustrated in Figure 3.16.



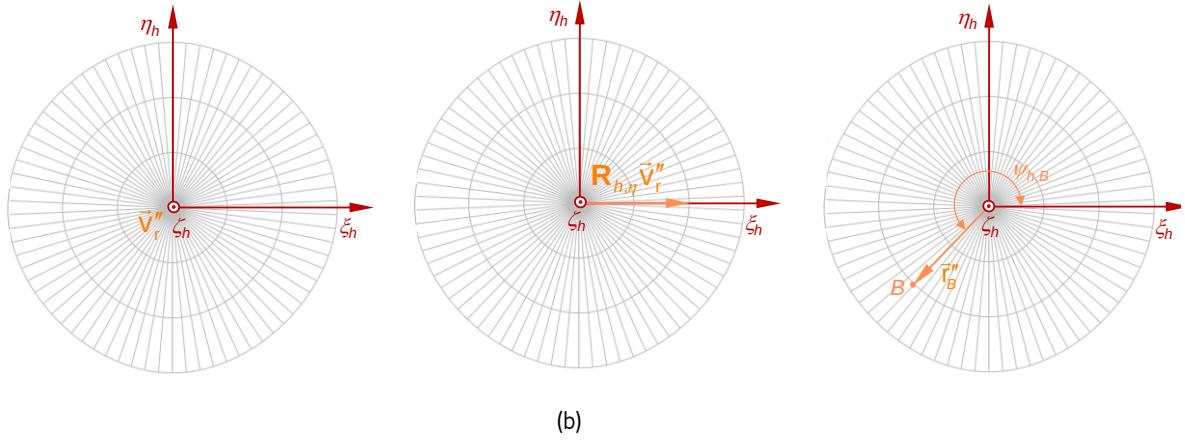


Figure 3.16 – Schematic representation of the transformation of vector $\mathbf{v}_r''$ into vector $\mathbf{r}_B''$. (a) Perspective and (b) top views.

Since the cone surface is fully defined by Eq. (3.53), the surface's tangent vectors, $\mathbf{t}_G''$ and $\mathbf{t}_\psi''$ can be calculated through the derivatives of vector $\mathbf{r}_B''$ with respect to G and $\psi_{h,B}$, respectively, as

$$\mathbf{t}_G'' = \begin{Bmatrix} \cos(\psi_{h,B}) \sin(\sigma_{h,\max,B}(\psi_{h,B})) \\ \sin(\psi_{h,B}) \sin(\sigma_{h,\max,B}(\psi_{h,B})) \\ \cos(\sigma_{h,\max,B}(\psi_{h,B})) \end{Bmatrix} \quad (3.54)$$

$$\mathbf{t}_\psi'' = \begin{Bmatrix} G \left(-\sin(\psi_{h,B}) \sin(\sigma_{h,\max,B}(\psi_{h,B})) + \cos(\psi_{h,B}) \cos(\sigma_{h,\max,B}(\psi_{h,B})) \frac{d\sigma_{h,\max,B}}{d\psi_{h,B}} \right) \\ G \left(\cos(\psi_{h,B}) \sin(\sigma_{h,\max,B}(\psi_{h,B})) + \sin(\psi_{h,B}) \cos(\sigma_{h,\max,B}(\psi_{h,B})) \frac{d\sigma_{h,\max,B}}{d\psi_{h,B}} \right) \\ G \left(-\sin(\sigma_{h,\max,B}(\psi_{h,B})) \frac{d\sigma_{h,\max,B}}{d\psi_{h,B}} \right) \end{Bmatrix} \quad (3.55)$$

where $\frac{d\sigma_{h,\max,B}}{d\psi_{h,B}}$ is the derivative of $\sigma_{h,\max,B}$ with respect to $\psi_{h,B}$. The value of $\frac{d\sigma_{h,\max,B}}{d\psi_{h,B}}$ depends on

whether the elliptical or the polynomial approach is considered, and, therefore, this parameter can be expressed, respectively, as

$$\frac{d\sigma_{h,\max,B}}{d\psi_{h,B}} = \frac{1}{a^2 b^2} (b^2 - a^2) \sin(\psi_{h,B}) \cos(\psi_{h,B}) \left(\frac{a^2 b^2 \frac{1}{\cos^2(\psi_{h,B})}}{a^2 \tan^2(\psi_{h,B}) + b^2} \right)^{3/2} \quad (3.56)$$

or

$$\frac{d\sigma_{h,\max,B}}{d\psi_{h,B}} = \frac{\partial\sigma_{h,\max,B}}{\partial\psi_{h,B}} = \frac{\partial\sigma_{h,\max,B}}{\partial l} \frac{\partial l}{\partial\psi_{h,B}} = \frac{\partial\sigma_{h,\max,B}}{\partial l} \left(\frac{\partial\psi_{h,B}}{\partial l} \right) \quad (3.57)$$

where

$$\frac{\partial\sigma_{h,\max,B}}{\partial l} = \frac{1}{\sqrt{x^2 + y^2}} \left((3c_{x,3}^k l^2 + 2c_{x,2}^k l + c_{x,1}^k) x + (3c_{y,3}^k l^2 + 2c_{y,2}^k l + c_{y,1}^k) y \right) \quad (3.58)$$

$$\frac{\partial\psi_{h,B}}{\partial l} = \frac{x^2}{y^2 + x^2} \left(\left(\frac{3c_{y,3}^k l^2 + 2c_{y,2}^k l + c_{y,1}^k}{x} \right) - \left(\frac{y(3c_{x,3}^k l^2 + 2c_{x,2}^k l + c_{x,1}^k)}{x^2} \right) \right) \quad (3.59)$$

in which x and y are given by Eqs. (3.47) and (3.48), respectively. In order to determine the expression of $\frac{d\sigma_{h,\max,B}}{d\psi_{h,B}}$ for the polynomial approach, Eq. (3.57), the inverse function rule must be utilized, which states that the derivative of the inverse function is the inverse of the derivative of the original function.

The vectors $\mathbf{t}_G''$ and $\mathbf{t}_\psi''$, given by Eqs. (3.54) and (3.55), are tangent to the surface of the circumduction cone along two different directions, namely along the generating line of the cone and along the perimeter of the base of the cone, respectively. A schematic representation of these two vectors is presented in Figure 3.17.

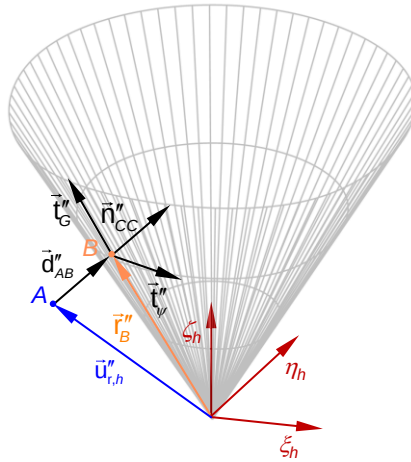


Figure 3.17 – Schematic representation of vectors $\mathbf{t}_G''$, $\mathbf{t}_\psi''$, $\mathbf{r}_B''$, $\mathbf{n}_{CC}''$, $\mathbf{d}_{AB}''$ and $\mathbf{u}_{r,h}''$ on an arbitrary circumduction cone.

In Figure 3.17, vector $\mathbf{n}_{CC}''$ represents the unit vector normal to the surface of the circumduction cone at point B for the corresponding value of $\sigma_{h,\max,B}$ and it is calculated as

$$\mathbf{n}_{CC}'' = \frac{\tilde{\mathbf{t}}_G'' \mathbf{t}_\psi''}{\|\tilde{\mathbf{t}}_G'' \mathbf{t}_\psi''\|} \quad (3.60)$$

The minimum distance condition is considered to determine point B , i.e., the closest point to A in the cone surface, and, consequently, the corresponding parameters G and ψ_h . This condition ensures

that the distance vector between points A and B , $\mathbf{d}_{AB}''$, and the normal vector to the surface of the circumduction cone at point B , $\mathbf{n}_{CC}''$, are collinear. Observing Figure 3.17, vector $\mathbf{d}_{AB}''$ is calculated as

$$\mathbf{d}_{AB}'' = \mathbf{r}_B'' - \mathbf{u}_{r,h}'' \quad (3.61)$$

The mathematical definition of two collinear vectors is given by their null cross product. In this methodology, the vectors tangent to the surface of the circumduction cone, $\mathbf{t}_G''$ and $\mathbf{t}_\psi''$, are utilized instead of the normal vector $\mathbf{n}_{CC}''$. Thus, the minimum distance condition must be modified. The cross product of vector $\mathbf{d}_{AB}''$ and a vector normal to the surface of the circumduction cone, $\mathbf{n}_{CC}''$, is equivalent to the inner products of vector $\mathbf{d}_{AB}''$ and the tangent vectors to the cone's surface as

$$\tilde{\mathbf{d}}_{AB}'' \mathbf{n}_{CC}'' = \mathbf{0} \Leftrightarrow \begin{cases} \mathbf{d}_{AB}''^T \mathbf{t}_G'' = 0 \\ \mathbf{d}_{AB}''^T \mathbf{t}_\psi'' = 0 \end{cases} \quad (3.62)$$

This set of nonlinear equations can be solved by using a root finding algorithm in order to obtain the set of parameters G and ψ_h at point B that satisfy the minimum distance condition. After knowing the longitude at point B , $\psi_{h,B}$, the corresponding maximum allowable latitude, $\sigma_{h,\max,B}$, can be calculated using the elliptical or polynomial approaches and Eqs. (3.44) or (3.49), respectively.

Moment Evaluation

In this work, the joint motion-restricting moment corresponds to a third-degree polynomial function with the behavior depicted in Figure 3.18, and it is expressed as (M. P. T. Silva et al., 1997)

$$\mathbf{m}_h''^{\text{mr}} = \begin{cases} \mathbf{0} & \text{if } \sigma_{h,A} \leq \sigma_{h,\max,A} \\ m_{\text{pe},h} \left[3 \left(\frac{\kappa}{\Delta\sigma_h} \right)^2 - 2 \left(\frac{\kappa}{\Delta\sigma_h} \right)^3 \right] \tilde{\mathbf{u}}_{r,h}'' \mathbf{n}_{CC}'' & \text{if } \sigma_{h,\max,A} < \sigma_{h,A} \text{ and } \kappa \leq \Delta\sigma_h \\ m_{\text{pe},h} \tilde{\mathbf{u}}_{r,h}'' \mathbf{n}_{CC}'' & \text{if } \kappa > \Delta\sigma_h \end{cases} \quad (3.63)$$

where $m_{\text{pe},h}$ is the magnitude of the maximum penalty moment applied to restrict the joint's motion, $\Delta\sigma_h$ corresponds to a quantity allowing to adjust the joint's stiffness and κ denotes the relative angular motion between the moving body and the limits of the circumduction cone. Parameter κ is calculated as the norm of the vector connecting point A to point B (see Figure 3.17) and it can be evaluated as

$$\kappa = \|\mathbf{d}_{AB}''\| = \sqrt{\sigma_{h,A}^2 + \sigma_{h,\max,B}^2 - 2\sigma_{h,A}\sigma_{h,\max,B} \cos(\psi_{h,A} - \psi_{h,B})} \quad (3.64)$$

It is important to note that the maximum magnitude defined for the joint-motion restricting moment, $m_{\text{pe},h}$, corresponds to the value at which the material of the joint reaches its yield limit.

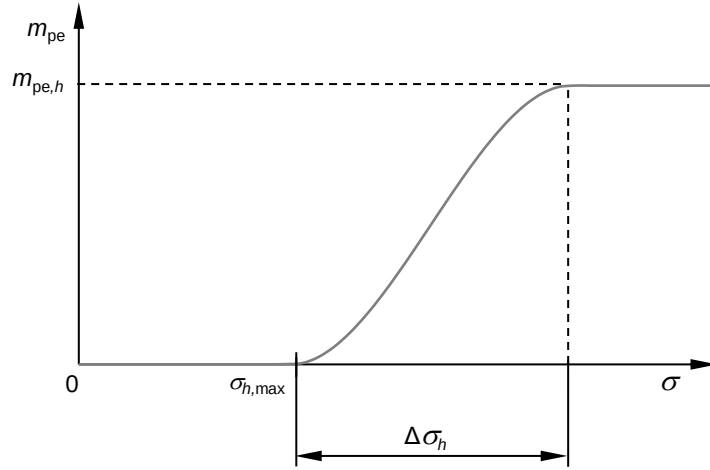


Figure 3.18 – Graphical representation of the nonlinear behavior of the joint motion-restricting moment.

The joint motion-restricting moment is calculated in the local coordinate system of the joint. In order to be applied to the reference and moving bodies, this moment must be expressed in global coordinates using Eq. (3.36). Finally, the expression (3.63) can easily be substituted by others existing in the literature (Nasr et al., 2023; Yamaguchi, 2001), or can be obtained by experimental testing, while keeping unchanged the remaining methodology described in the previous paragraphs.

3.3.2. Joint Dissipative Moment

In order to simulate the dissipative behavior of the materials constituent of mechanical joints and to allow energy dissipation, a joint dissipative moment is introduced in the presented formulation. The joint dissipative moment is calculated considering a viscous torsional damper as

$$\mathbf{m}_h^d = -j_h \boldsymbol{\omega}_h \quad (3.65)$$

where j_h is the rotational damping coefficient of the mechanical joint and $\boldsymbol{\omega}_h$ represents the joint h angular velocity vector, which is calculated as (see Figure 3.6)

$$\boldsymbol{\omega}_h = \boldsymbol{\omega}_j - \boldsymbol{\omega}_i \quad (3.66)$$

3.3.3. Flowchart of the Proposed Methodology

A flowchart of the methodology to restrict the RoM of mechanical joints proposed in this work is presented in Figure 3.19 and it can be summarized by the following steps:

1. Start, at the initial configuration, by defining the input parameters, namely
 - 1.1. Unit vectors defining the ξ and η axis of the joint h local coordinate system expressed in local coordinates of the reference body, $\mathbf{u}'_{\xi,h}$ and $\mathbf{u}'_{\eta,h}$;

- 1.2. Unit vector $\mathbf{u}_r$ expressed in local coordinates of the moving body, $\mathbf{u}'_{r,h}$;
- 1.3. Longitude, ψ_h , and maximum allowable latitude, $\sigma_{h,\max}$, vectors of joint h ;
- 1.4. Maximum joint motion-restricting moment magnitude, $m_{pe,h}$;
- 1.5. Damping coefficient of joint h , j_h ;
- 1.6. Compliance of joint h , $\Delta\sigma_h$.
2. Calculate the joint dissipative moment, $\mathbf{m}_h^d$, using Eq. (3.65).
3. Evaluate the following
 - 3.1. Unit vectors $\mathbf{u}'_{\xi,h}$, $\mathbf{u}'_{\eta,h}$ and $\mathbf{u}'_{r,h}$ expressed in global coordinates using an expression similar to Eq. (3.21);
 - 3.2. Joint local coordinate system using Eq. (3.35);
 - 3.3. Unit vector $\mathbf{u}_r$ expressed in the joint local coordinate system utilizing Eq. (3.36);
 - 3.4. Longitude, $\psi_{h,A}$, and latitude, $\sigma_{h,A}$, at point A , using Eqs. (3.37) and (3.38).
4. Assess the maximum allowable latitude at point A , $\sigma_{h,\max,A}$, applying either the elliptical or the polynomial approaches and Eqs. (3.44) and (3.49), respectively.
5. If the current latitude at point A , $\sigma_{h,A}$, does not exceed the maximum allowable latitude, $\sigma_{h,\max,A}$, for the corresponding longitude, $\psi_{h,A}$, the joint motion-restricting moment is null.
6. If the current latitude at point A , $\sigma_{h,A}$, exceeds the maximum allowable latitude, $\sigma_{h,\max,A}$, for the corresponding longitude, $\psi_{h,A}$, the following steps should be taken
 - 6.1. Solve a system of nonlinear equations for G and $\psi_{h,B}$ using Eq. (3.62).
 - 6.2. Assess the maximum allowable latitude at point B , $\sigma_{h,\max,B}$, applying either the elliptical or polynomial approaches and Eqs. (3.44) and (3.49), respectively.
 - 6.3. Calculate the joint motion-restricting moment in local coordinates of the joint coordinate system, $\mathbf{m}_h^{\text{mr}}$, using Eq. (3.63);
 - 6.4. Evaluate the joint motion-restricting moment in global coordinates, $\mathbf{m}_h^{\text{mr}}$, using Eq. (3.36);
7. Calculate the joint resistance moments, $\mathbf{m}_h^r$, using Eq. (3.34) and apply them to the connected bodies.
8. Proceed with the process described in steps 1-7 for a new time step until the final time of analysis is reached.

The joint resistance moments constitute an action-reaction pair and, thus, the results obtained using Eq. (3.34) are applied on the moving body and their symmetrical are applied on the reference body.

In the multibody systems methodology, these moments are taken as external moments integrated in vector $\mathbf{g}$ of Eq. (3.14), which contains all the external generalized forces acting on the system (P. Nikravesh, 1988; M. R. Silva et al., 2024b).

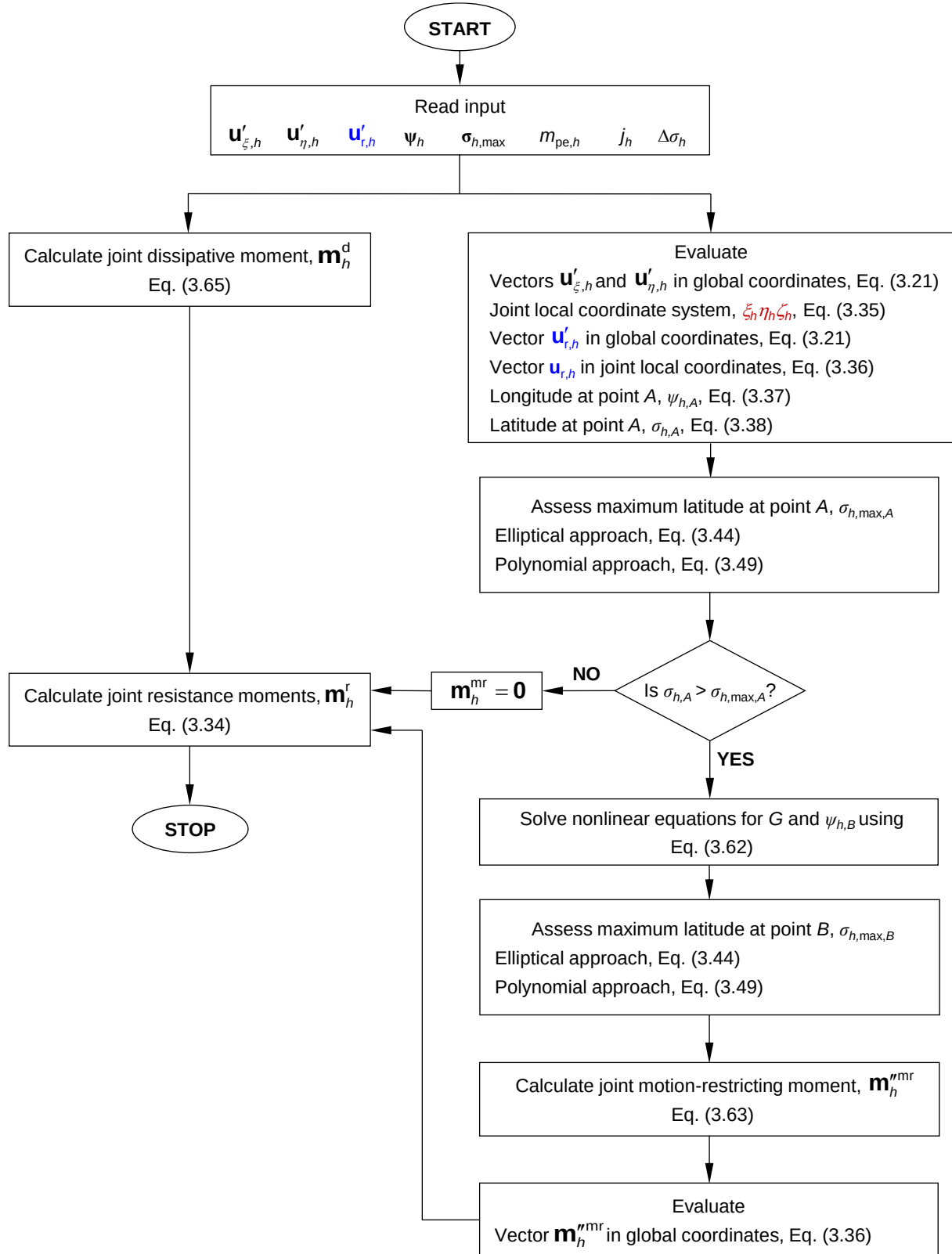


Figure 3.19 – Flowchart of the improved methodology proposed in this work.

3.4. Formulation of the Driving Constraints

Driving or guiding constraints are a type of rheonomic constraints that are utilized to guide the degrees-of-freedom of multibody systems. The driving constraints are expressed as functions of the time variable and, in biomechanics of motion, are usually obtained experimentally by using an optoelectronic motion capture system. The experimental data is typically discrete, and it is utilized to derive the mathematical expressions by interpolating the driving variables along the time of the analysis (P. Nikravesh, 1988). This procedure can be accomplished by using either cubic or higher-order splines interpolation. However, higher-order splines tend to swing through wild oscillations in the vicinity of an abrupt change, whereas cubic splines provides smoother transitions. Furthermore, cubic splines are helpful to ensure the continuity of the first and second derivatives, velocity, and acceleration, respectively, property that is crucial in kinematic and dynamic analyses (Chapra & Canale, 1989; Späth, 1995).

The formulation developed in this work to prescribe the experimental data to the biomechanical model considers five types of driving constraints, namely guiding (i) a generic point G , (ii) an arbitrary Euler parameter, (iii) the angle between two vectors $\mathbf{a}_i$ and $\mathbf{b}_j$, (iv) the angle between a vector $\mathbf{a}_i$ and a massless link vector $\mathbf{d}$ and (v) the angle between a vector $\mathbf{a}_i$ and a vector projected on a plane $\mathbf{b}_{j,p}$. The first and second driving constraints allow to control the trajectory and orientation of a body, respectively. A detailed description of the developed driving constraints is provided in the following paragraphs.

In order to guide a generic point G , the following three kinematic constraint equations must be considered (see Figure 3.20)

$$\Phi^{(G,3)} \equiv \mathbf{r}_i^G - \mathbf{c}^*(t) = \mathbf{r}_i + \mathbf{s}_i^G - \mathbf{c}^*(t) = \mathbf{0} \quad (3.67)$$

in which $\mathbf{c}^*(t)$ is the prescribed experimental data containing the x , y , and z coordinates of the guided point G , $\mathbf{r}_i^G$ represents the global position vector of point G located on body i , $\mathbf{r}_i$ is the position vector of the center of mass of body i described in global coordinates, and $\mathbf{s}_i^G$ represents the global position vector of point G located on body i with respect to the body's local coordinate system. The local and global components of vector $\mathbf{s}_i^G$ are related to each other using an expression similar to Eq. (3.21).

The velocity constraint equations for this driving constraint can be obtained by taking the first time derivative of Eq. (3.67), yielding

$$\dot{\Phi}^{(G,3)} \equiv \dot{\mathbf{r}}_i + \dot{\mathbf{s}}_i^G - \dot{\mathbf{c}}^*(t) = \mathbf{0} \quad (3.68)$$

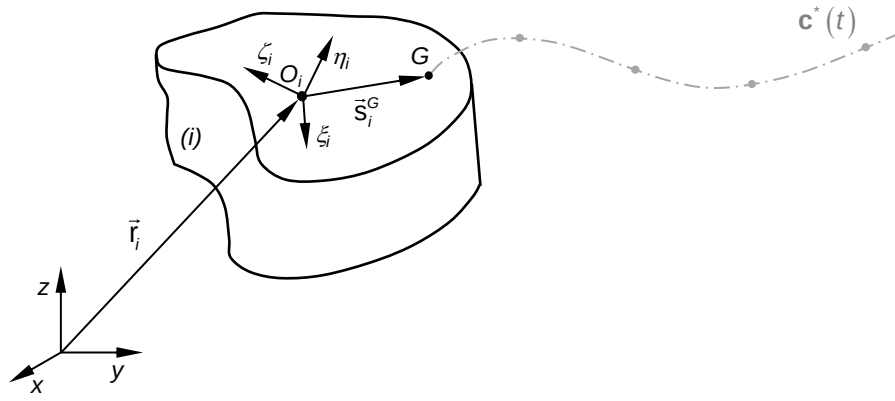


Figure 3.20 – Schematic representation of a body i with prescribed trajectory for a generic point G .

Equation (3.68) is not explicitly expressed in terms of the angular velocity of body i , which is necessary to establish the Jacobian matrix, and, therefore, Eq. (3.27) should be considered. Equation (3.68) can be rewritten as

$$\dot{\Phi}^{(G,3)} \equiv \dot{\mathbf{r}}_i - \tilde{\mathbf{s}}_i^G \boldsymbol{\omega}_i - \dot{\mathbf{c}}^*(t) = \mathbf{0} \quad (3.69)$$

Observing Eq. (3.69), the contribution to the Jacobian matrix of the constraint equations to guide a generic point G can be expressed as

$$\mathbf{D}^{(G,3)} = [\mathbf{I} \quad -\tilde{\mathbf{s}}_i^G] \quad (3.70)$$

in which $\mathbf{I}$ represents the identity matrix.

The formulation of the driving constraints considered in this work is an explicit function of time, and, consequently, the right-hand side vector of the velocity constraint equations, $\mathbf{v}$, is not null. For the case presented in Eq. (3.69), vector $\mathbf{v}$ is expressed as

$$\mathbf{v}^{(G,3)} = -\frac{\partial \Phi^{(G,3)}}{\partial t} = \dot{\mathbf{c}}^*(t) \quad (3.71)$$

The second time derivative of Eq. (3.67) yields the acceleration constraint equations as

$$\ddot{\Phi}^{(G,3)} \equiv \ddot{\mathbf{r}}_i + \ddot{\mathbf{s}}_i^G - \ddot{\mathbf{c}}^*(t) = \mathbf{0} \quad (3.72)$$

Equation (3.72) is not expressed in terms of the angular acceleration of body i , which is necessary to establish the right-hand side vector of the acceleration equations. Hence, considering the condition expressed in Eq. (3.31), Eq. (3.72) can be rewritten as

$$\ddot{\Phi}^{(G,3)} \equiv \ddot{\mathbf{r}}_i - \tilde{\mathbf{s}}_i^G \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i^G - \ddot{\mathbf{c}}^*(t) = \mathbf{0} \quad (3.73)$$

Observing Eq. (3.73), the contribution of the first type of driving constraints to the right-hand side of the acceleration equations can be established as

$$\boldsymbol{\gamma}^{(G,3)} = \ddot{\mathbf{c}}^*(t) - \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i^G \quad (3.74)$$

The second formulation developed to prescribe the experimental data to the biomechanical model is to guide one arbitrary Euler parameter, e_k ($k = 0, 1, 2, 3$) using the following driving constraint equation

$$\Phi^{(e_k,1)} \equiv e_k - e_k^*(t) = 0 \quad (3.75)$$

where $e_k^*(t)$ is the experimental data for e_k .

The velocity constraint equation for this driving constraint is obtained by taking the first time derivative of Eq. (3.75) yielding

$$\dot{\Phi}^{(e_k,1)} \equiv \dot{e}_k - \dot{e}_k^*(t) = 0 \quad (3.76)$$

Equation (3.76) can be rearranged to include the expression of the time derivative of the Euler parameters as

$$\dot{\Phi}^{(e_k,1)} \equiv \frac{1}{2} \left(\mathbf{G}_{(1:3,k+1)} \right)^T \boldsymbol{\omega}_i - \dot{e}_k^*(t) = 0 \quad (3.77)$$

in which $\mathbf{G}$ represents the transformation matrix in terms of the Euler parameters (P. Nikravesh, 1988).

Observing Eq. (3.77), the Jacobian matrix of the driving constraint equation formulated in Eq. (3.75) is expressed as

$$\mathbf{D}^{(e_k,1)} = \left[\mathbf{0} \quad \frac{1}{2} \left(\mathbf{G}_{(1:3,k+1)} \right)^T \right] \quad (3.78)$$

and the right-hand side vector of the velocity constraint equations is established as

$$\mathbf{v}^{(e_k,1)} = -\frac{\partial \Phi^{(e_k,1)}}{\partial t} = \dot{e}_k^*(t) \quad (3.79)$$

The time derivative of Eq. (3.77) yields the acceleration constraint equation of the driving constraint to guide an arbitrary Euler parameter as

$$\ddot{\Phi}^{(e_k,1)} \equiv \frac{1}{2} \boldsymbol{\omega}_i^T \dot{\mathbf{G}}_{(1:3,k+1)} + \frac{1}{2} \left(\mathbf{G}_{(1:3,k+1)} \right)^T \dot{\boldsymbol{\omega}}_i - \ddot{e}_k^*(t) = 0 \quad (3.80)$$

Thus, the contribution of Eq. (3.75) to the right-hand side of the acceleration equations yields

$$\gamma^{(e_k,1)} = \ddot{e}_k^*(t) - \frac{1}{2} \boldsymbol{\omega}_i^T \dot{\mathbf{G}}_{(1:3,k+1)} \quad (3.81)$$

In order to guide the angle between two arbitrary $\mathbf{a}_i$ and $\mathbf{b}_j$ vectors, belonging to bodies i and j , respectively, the following driving constraint equation must be formulated (see Figure 3.21)

$$\Phi^{(\theta,1)} \equiv \mathbf{a}_i^T \mathbf{b}_j - \cos \theta^*(t) = 0 \quad (3.82)$$

where $\theta^*(t)$ is the angle between the $\mathbf{a}_i$ and $\mathbf{b}_j$ vectors calculated using the experimental data. Vectors $\mathbf{a}_i$ and $\mathbf{b}_j$ must be unit vectors perpendicular to the joint axis $\mathbf{s}_k$ ($k = i, j$) expressed in global coordinates.

The constraint Eq. (3.82) is utilized to guide the angle of revolute and classical universal joints.

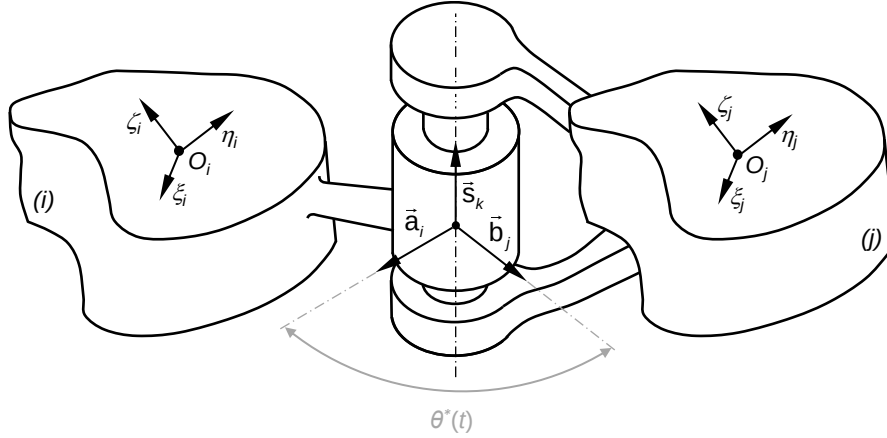


Figure 3.21 – Schematic representation of bodies i and j connected by a revolute joint with axis $\bar{s}_k$ ($k = i, j$). The angle $\theta^*(t)$ between the two arbitrary $\bar{a}_i$ and $\bar{b}_j$ unit vectors is prescribed using experimental data.

The first time derivative of Eq. (3.82) yields the velocity constraint equation as

$$\dot{\Phi}^{(\theta,1)} \equiv \bar{\mathbf{b}}_j^T \dot{\bar{\mathbf{a}}}_i + \bar{\mathbf{a}}_i^T \dot{\bar{\mathbf{b}}}_j + \sin \theta^*(t) \dot{\theta}^*(t) = 0 \quad (3.83)$$

Using the condition expressed in Eq. (3.27), Eq. (3.83) can be rewritten as

$$\dot{\Phi}^{(\theta,1)} \equiv -\bar{\mathbf{b}}_j^T \tilde{\mathbf{a}}_i \boldsymbol{\omega}_i - \bar{\mathbf{a}}_i^T \tilde{\mathbf{b}}_j \boldsymbol{\omega}_j + \sin \theta^*(t) \dot{\theta}^*(t) = 0 \quad (3.84)$$

Observing Eq. (3.84), the Jacobian matrix and right-hand side vector of the velocity constraint equations for the constraint to guide the angle between two arbitrary $\bar{\mathbf{a}}_i$ and $\bar{\mathbf{b}}_j$ unit vectors can be established, respectively, as

$$\mathbf{D}^{(\theta,1)} = \begin{bmatrix} \mathbf{0} & -\bar{\mathbf{b}}_j^T \tilde{\mathbf{a}}_i & \mathbf{0} & -\bar{\mathbf{a}}_i^T \tilde{\mathbf{b}}_j \end{bmatrix} \quad (3.85)$$

$$\mathbf{v}^{(\theta,1)} = -\frac{\partial \Phi^{(\theta,1)}}{\partial t} = -\sin \theta^*(t) \dot{\theta}^*(t) \quad (3.86)$$

The time derivative of Eq. (3.83) yields the acceleration constraint equation as

$$\ddot{\Phi}^{(\theta,1)} \equiv \bar{\mathbf{b}}_j^T \ddot{\bar{\mathbf{a}}}_i + \bar{\mathbf{a}}_i^T \ddot{\bar{\mathbf{b}}}_j + 2\dot{\bar{\mathbf{a}}}_i^T \dot{\bar{\mathbf{b}}}_j + \cos \theta^*(t) \dot{\theta}^*(t)^2 + \sin \theta^*(t) \ddot{\theta}^*(t) = 0 \quad (3.87)$$

Taking advantage of Eq. (3.31), then Eq. (3.87) becomes

$$\begin{aligned} \ddot{\Phi}^{(\theta,1)} \equiv & -\bar{\mathbf{b}}_j^T \tilde{\boldsymbol{\omega}}_i \dot{\bar{\mathbf{a}}}_i + \bar{\mathbf{b}}_j^T \tilde{\boldsymbol{\omega}}_i \dot{\bar{\mathbf{a}}}_i - \bar{\mathbf{a}}_i^T \tilde{\boldsymbol{\omega}}_j \dot{\bar{\mathbf{b}}}_j + \bar{\mathbf{a}}_i^T \tilde{\boldsymbol{\omega}}_j \dot{\bar{\mathbf{b}}}_j + 2\dot{\bar{\mathbf{a}}}_i^T \dot{\bar{\mathbf{b}}}_j \\ & + \cos \theta^*(t) \dot{\theta}^*(t)^2 + \sin \theta^*(t) \ddot{\theta}^*(t) = 0 \end{aligned} \quad (3.88)$$

Thus, the contribution of the driving constraint (3.82) to the right-hand side vector of the accelerations is as

$$\gamma^{(\theta,1)} = -\bar{\mathbf{b}}_j^T \tilde{\boldsymbol{\omega}}_i \dot{\bar{\mathbf{a}}}_i - \bar{\mathbf{a}}_i^T \tilde{\boldsymbol{\omega}}_j \dot{\bar{\mathbf{b}}}_j - 2\dot{\bar{\mathbf{a}}}_i^T \dot{\bar{\mathbf{b}}}_j - \cos \theta^*(t) \dot{\theta}^*(t)^2 - \sin \theta^*(t) \ddot{\theta}^*(t) \quad (3.89)$$

The fourth driving constraint is utilized to guide the angle of each joint of the modified universal joint (see Figure 3.5b). In order to correctly calculate the joint angle in a modified universal joint, the massless link vector must be projected onto the plane perpendicular to the $\mathbf{s}_i$ joint axis, $\mathbf{d}_p$. If vector $\mathbf{d}$ is utilized instead of vector $\mathbf{d}_p$, a joint angle resulting from the combination of the rotation about the axes of both joints at a specific configuration would be guided, instead of the real angle corresponding to the rotation about only one joint axis. Vector $\mathbf{d}_p$ is established as

$$\mathbf{d}_p = \mathbf{d} - (\mathbf{d}^T \mathbf{s}_i) \mathbf{s}_i \quad (3.90)$$

The kinematic constraint equation developed to guide the angle between one arbitrary unit vector $\mathbf{a}_i$ perpendicular to the $\mathbf{s}_i$ joint axis and the projected massless link $\mathbf{d}_p$ is expressed as

$$\Phi^{(\varphi,1)} \equiv \frac{\mathbf{a}_i^T \mathbf{d}_p}{\|\mathbf{d}_p\|} - \cos \varphi^*(t) = 0 \quad (3.91)$$

in which $\varphi^*(t)$ is the angle between the $\mathbf{a}_i$ and $\mathbf{d}_p$ vectors calculated using the experimental data. It must be noted that the vector $\mathbf{a}_i$ belongs to body i and it must be a unit vector. A schematic representation of vectors $\mathbf{d}$, $\mathbf{d}_p$ and $\mathbf{a}_i$ for one joint axis of the modified universal joint is depicted in Figure 3.22.

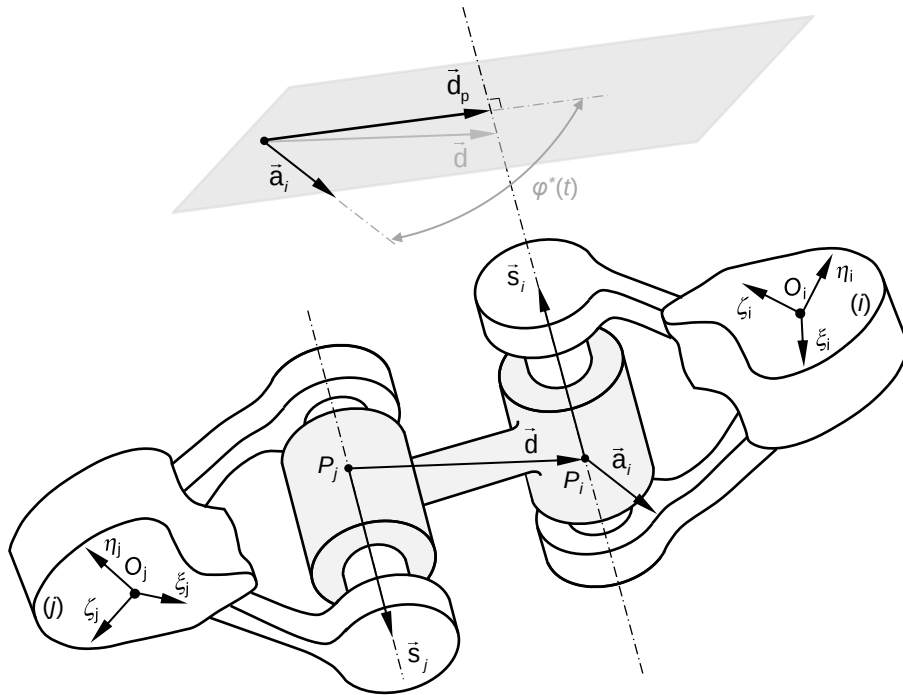


Figure 3.22 – Schematic representation of a modified universal joint with vectors $\mathbf{d}$, $\mathbf{d}_p$ and $\mathbf{a}_i$. The angle $\varphi^*(t)$ is prescribed using experimental data.

The velocity constraint equation is obtained by taking the first time derivative of Eq. (3.91) as

$$\dot{\Phi}^{(\varphi,1)} \equiv \frac{1}{\|\mathbf{d}_p\|} (\mathbf{d}_p^T \dot{\mathbf{a}}_i + \mathbf{a}_i^T \dot{\mathbf{d}}_p) + \sin \varphi^*(t) \dot{\varphi}^*(t) = 0 \quad (3.92)$$

in which the first time derivative of vector $\mathbf{d}_p$ is established as

$$\dot{\mathbf{d}}_p = \dot{\mathbf{d}} - \mathbf{s}_i^T \dot{\mathbf{d}} \mathbf{s}_i - \mathbf{d}^T \dot{\mathbf{s}}_i \mathbf{s}_i - \mathbf{d}^T \mathbf{s}_i \dot{\mathbf{s}}_i \quad (3.93)$$

and the first time derivative of vector $\mathbf{d}$ is defined as

$$\dot{\mathbf{d}} = \dot{\mathbf{r}}_j + \dot{\mathbf{s}}_j^P - \dot{\mathbf{r}}_i - \dot{\mathbf{s}}_i^P \quad (3.94)$$

Making use of Eq. (3.27), then Eq. (3.92) becomes

$$\begin{aligned} \dot{\Phi}^{(\varphi,1)} \equiv & \frac{1}{\|\mathbf{d}_p\|} \left(\mathbf{a}_i^T (\mathbf{s}_i \mathbf{s}_i^T - \mathbf{I}) \dot{\mathbf{r}}_i + \left(-\mathbf{d}_p^T \tilde{\mathbf{a}}_i + \mathbf{a}_i^T (\tilde{\mathbf{s}}_i^P - \mathbf{s}_i \mathbf{s}_i^T \tilde{\mathbf{s}}_i^P + \mathbf{s}_i \mathbf{d}^T \tilde{\mathbf{s}}_i + \mathbf{d}^T \mathbf{s}_i \tilde{\mathbf{s}}_i) \right) \boldsymbol{\omega}_i \right. \\ & \left. + \mathbf{a}_i^T (\mathbf{I} - \mathbf{s}_i \mathbf{s}_i^T) \dot{\mathbf{r}}_j + \mathbf{a}_i^T (\mathbf{s}_i \mathbf{s}_i^T \tilde{\mathbf{s}}_j^P - \tilde{\mathbf{s}}_j^P) \boldsymbol{\omega}_j \right) + \sin \varphi^*(t) \dot{\varphi}^*(t) = 0 \end{aligned} \quad (3.95)$$

Thus, the corresponding contribution of the driving constraint (3.91) to the Jacobian matrix and to the right-hand side vector of the velocities can be expressed, respectively, as

$$\mathbf{D}^{(\varphi,1)} = \begin{bmatrix} \frac{\mathbf{a}_i^T (\mathbf{s}_i \mathbf{s}_i^T - \mathbf{I})}{\|\mathbf{d}_p\|} & \frac{-\mathbf{d}_p^T \tilde{\mathbf{a}}_i + \mathbf{a}_i^T (\tilde{\mathbf{s}}_i^P - \mathbf{s}_i \mathbf{s}_i^T \tilde{\mathbf{s}}_i^P + \mathbf{s}_i \mathbf{d}^T \tilde{\mathbf{s}}_i + \mathbf{d}^T \mathbf{s}_i \tilde{\mathbf{s}}_i)}{\|\mathbf{d}_p\|} & \frac{\mathbf{a}_i^T (\mathbf{I} - \mathbf{s}_i \mathbf{s}_i^T)}{\|\mathbf{d}_p\|} & \frac{\mathbf{a}_i^T (\mathbf{s}_i \mathbf{s}_i^T \tilde{\mathbf{s}}_j^P - \tilde{\mathbf{s}}_j^P)}{\|\mathbf{d}_p\|} \end{bmatrix} \quad (3.96)$$

$$\mathbf{v}^{(\varphi,1)} = -\frac{\partial \Phi^{(\varphi,1)}}{\partial t} = -\sin \varphi^*(t) \dot{\varphi}^*(t) \quad (3.97)$$

The time derivative of Eq. (3.92) yields the acceleration constraint equations as

$$\ddot{\Phi}^{(\varphi,1)} \equiv \frac{1}{\|\mathbf{d}_p\|} \left(\dot{\mathbf{a}}_i^T \dot{\mathbf{d}}_p + \mathbf{d}_p^T \ddot{\mathbf{a}}_i + \dot{\mathbf{d}}_p^T \ddot{\mathbf{a}}_i + \mathbf{a}_i^T \ddot{\mathbf{d}}_p \right) + \cos \varphi^*(t) \dot{\varphi}^*(t)^2 + \sin \varphi^*(t) \ddot{\varphi}^*(t) = 0 \quad (3.98)$$

in which the second time derivative of vector $\mathbf{d}_p$ is established as

$$\ddot{\mathbf{d}}_p = \ddot{\mathbf{d}} - \dot{\mathbf{d}}^T \dot{\mathbf{s}}_i \mathbf{s}_i - \mathbf{s}_i^T \ddot{\mathbf{d}} \mathbf{s}_i - \mathbf{s}_i^T \dot{\mathbf{d}} \dot{\mathbf{s}}_i - \dot{\mathbf{s}}_i^T \dot{\mathbf{d}} \mathbf{s}_i - \mathbf{d}^T \ddot{\mathbf{s}}_i \mathbf{s}_i - \mathbf{d}^T \dot{\mathbf{s}}_i \dot{\mathbf{s}}_i - \mathbf{s}_i^T \ddot{\mathbf{d}} \mathbf{s}_i - \mathbf{d}^T \dot{\mathbf{s}}_i \dot{\mathbf{s}}_i - \mathbf{d}^T \mathbf{s}_i \ddot{\mathbf{s}}_i \quad (3.99)$$

and the second time derivative of vector $\mathbf{d}$ is calculated as

$$\ddot{\mathbf{d}} = \ddot{\mathbf{r}}_j + \ddot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i - \ddot{\mathbf{s}}_i^P \quad (3.100)$$

Taking into consideration the condition expressed in Eq. (3.31), then Eq. (3.98) is rewritten as

$$\begin{aligned} \ddot{\Phi}^{(\varphi,1)} \equiv & \frac{1}{\|\mathbf{d}_p\|} \left(2\dot{\mathbf{a}}_i^T \dot{\mathbf{d}}_p + \mathbf{d}_p^T (-\tilde{\mathbf{a}}_i \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{a}}_i) + \mathbf{a}_i^T (\ddot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i + \tilde{\mathbf{s}}_i^P \dot{\boldsymbol{\omega}}_i - \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i^P \right. \\ & - \dot{\mathbf{d}}^T \dot{\mathbf{s}}_i \mathbf{s}_i - \mathbf{s}_i^T \ddot{\mathbf{r}}_j \mathbf{s}_i - \mathbf{s}_i^T (-\tilde{\mathbf{s}}_j^P \dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{s}}_j^P) \mathbf{s}_i + \mathbf{s}_i^T \ddot{\mathbf{r}}_i \mathbf{s}_i + \mathbf{s}_i^T (-\tilde{\mathbf{s}}_i^P \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i^P) \mathbf{s}_i - \mathbf{s}_i^T \dot{\mathbf{d}} \dot{\mathbf{s}}_i \\ & - \dot{\mathbf{s}}_i^T \dot{\mathbf{d}} \mathbf{s}_i - \mathbf{d}^T (-\tilde{\mathbf{s}}_i \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i) \mathbf{s}_i - 2\mathbf{d}^T \dot{\mathbf{s}}_i \dot{\mathbf{s}}_i - \mathbf{s}_i^T \ddot{\mathbf{d}} \mathbf{s}_i - \mathbf{d}^T \mathbf{s}_i (-\tilde{\mathbf{s}}_i \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i) \left. \right) \\ & - \cos \varphi^*(t) \dot{\varphi}^*(t)^2 - \sin \varphi^*(t) \ddot{\varphi}^*(t) = 0 \end{aligned} \quad (3.101)$$

Observing Eq. (3.101), the contribution to the right-hand side of the acceleration equations of the driving constraint (3.91) can be established as

$$\begin{aligned} \gamma^{(\phi,1)} = & \frac{1}{\|\mathbf{d}_p\|} \left(-2\dot{\mathbf{a}}_i^T \dot{\mathbf{d}}_p - \mathbf{d}_p^T \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{a}}_i - \mathbf{a}_i^T \left(\tilde{\boldsymbol{\omega}}_j \dot{\mathbf{s}}_j^P - \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i^P - \dot{\mathbf{d}}^T \dot{\mathbf{s}}_i \mathbf{s}_i - \mathbf{s}_i^T \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{s}}_j^P \right. \right. \\ & \left. \left. + \mathbf{s}_i^T \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i^P \mathbf{s}_i - \mathbf{s}_i^T \dot{\mathbf{d}} \dot{\mathbf{s}}_i - \dot{\mathbf{s}}_i^T \dot{\mathbf{d}} \mathbf{s}_i - \mathbf{d}^T \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i \mathbf{s}_i - 2\mathbf{d}^T \dot{\mathbf{s}}_i \dot{\mathbf{s}}_i - \mathbf{s}_i^T \dot{\mathbf{d}} \dot{\mathbf{s}}_i - \mathbf{d}^T \mathbf{s}_i \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i \right) \right) \\ & - \cos \phi^*(t) \dot{\phi}^*(t)^2 - \sin \phi^*(t) \ddot{\phi}^*(t) \end{aligned} \quad (3.102)$$

Finally, to guide each degree-of-freedom of a spherical joint independently, an additional driving constraint that allows to guide the angle between a vector $\mathbf{a}_i$ and a vector $\mathbf{b}_j$ projected onto a plane must be formulated. This driving constraint is specifically formulated for the biomechanical multibody model developed in Chapter 5, in which vector $\mathbf{b}_j$ must be projected on each cardinal plane to correctly estimate the flexion-extension, adduction-abduction, and internal and external rotation angles of the spherical joint in the sagittal, frontal, and transverse planes, respectively. The last developed driving constraint is formulated as (see Figure 3.23)

$$\phi^{(\phi,1)} \equiv \frac{\mathbf{a}_i^T \mathbf{b}_{j,p}}{\|\mathbf{b}_{j,p}\|} - \cos \phi^*(t) = 0 \quad (3.103)$$

in which $\phi^*(t)$ is the angle between the $\mathbf{a}_i$ and $\mathbf{b}_{j,p}$ vectors calculated using the experimental data, vector $\mathbf{b}_{j,p}$ is established as

$$\mathbf{b}_{j,p} = \mathbf{b}_j - (\mathbf{b}_j^T \mathbf{s}_i) \mathbf{s}_i \quad (3.104)$$

where $\mathbf{s}_i$ represents a vector perpendicular to the plane on which vector $\mathbf{b}_{j,p}$ is projected, and the norm of vector $\mathbf{b}_{j,p}$ is defined as

$$\|\mathbf{b}_{j,p}\| = (\mathbf{b}_{j,p}^T \mathbf{b}_{j,p})^{\frac{1}{2}} \quad (3.105)$$

It is important to note that the vectors $\mathbf{a}_i$ and $\mathbf{s}_i$ must be unit vectors.

The first time derivative of Eq. (3.103) yields the velocity constraint equation as

$$\dot{\phi}^{(\phi,1)} \equiv \frac{\|\mathbf{b}_{j,p}\| (\mathbf{b}_{j,p}^T \dot{\mathbf{a}}_i + \mathbf{a}_i^T \dot{\mathbf{b}}_{j,p}) - (\mathbf{a}_i^T \mathbf{b}_{j,p}) \|\dot{\mathbf{b}}_{j,p}\|}{\|\mathbf{b}_{j,p}\|^2} + \sin \phi^*(t) \dot{\phi}^*(t) = 0 \quad (3.106)$$

in which the time derivative of the norm of vector $\mathbf{b}_{j,p}$ is established as

$$\|\dot{\mathbf{b}}_{j,p}\| = \frac{1}{\|\mathbf{b}_{j,p}\|} (\mathbf{b}_{j,p}^T \dot{\mathbf{b}}_{j,p}) \quad (3.107)$$

Substituting Eq. (3.107) into Eq. (3.106), yields

$$\dot{\phi}^{(\phi,1)} \equiv \frac{\|\mathbf{b}_{j,p}\|^2 (\mathbf{b}_{j,p}^T \dot{\mathbf{a}}_i + \mathbf{a}_i^T \dot{\mathbf{b}}_{j,p}) - (\mathbf{a}_i^T \mathbf{b}_{j,p}) (\mathbf{b}_{j,p}^T \dot{\mathbf{b}}_{j,p})}{\|\mathbf{b}_{j,p}\|^3} + \sin \phi^*(t) \dot{\phi}^*(t) = 0 \quad (3.108)$$

where the first time derivative of vector $\mathbf{b}_{j,p}$ is established as

$$\dot{\mathbf{b}}_{j,p} = \dot{\mathbf{b}}_j - \mathbf{s}_i^T \dot{\mathbf{b}}_j \mathbf{s}_i - \mathbf{b}_j^T \dot{\mathbf{s}}_i \mathbf{s}_i - \mathbf{b}_j^T \mathbf{s}_i \dot{\mathbf{s}}_i \quad (3.109)$$

Applying Eq. (3.27), then Eq. (3.108) becomes

$$\begin{aligned} \dot{\Phi}^{(\phi,1)} \equiv & \frac{1}{\|\mathbf{b}_{j,p}\|^3} \left(\|\mathbf{b}_{j,p}\|^2 \left(-\mathbf{b}_{j,p}^T \tilde{\mathbf{a}}_i \boldsymbol{\omega}_i + \mathbf{a}_i^T \left(-\tilde{\mathbf{b}}_j \boldsymbol{\omega}_j + \mathbf{s}_i \mathbf{s}_i^T \tilde{\mathbf{b}}_j \boldsymbol{\omega}_j + \mathbf{s}_i \mathbf{b}_j^T \tilde{\mathbf{s}}_i \boldsymbol{\omega}_i + \mathbf{b}_j^T \mathbf{s}_i \tilde{\mathbf{s}}_i \boldsymbol{\omega}_i \right) \right) \right. \\ & \left. - \left(\mathbf{a}_i^T \mathbf{b}_{j,p} \right) \left(\mathbf{b}_{j,p}^T \left(-\tilde{\mathbf{b}}_j \boldsymbol{\omega}_j + \mathbf{s}_i \mathbf{s}_i^T \tilde{\mathbf{b}}_j \boldsymbol{\omega}_j + \mathbf{s}_i \mathbf{b}_j^T \tilde{\mathbf{s}}_i \boldsymbol{\omega}_i + \mathbf{b}_j^T \mathbf{s}_i \tilde{\mathbf{s}}_i \boldsymbol{\omega}_i \right) \right) \right) + \sin \phi^*(t) \dot{\phi}^*(t) = 0 \end{aligned} \quad (3.110)$$

Thus, observing Eq. (3.110), the contribution of the driving constraint (3.103) to the Jacobian matrix can be expressed as

$$\mathbf{D}^{(\phi,1)} = \frac{1}{\|\mathbf{b}_{j,p}\|^3} [\mathbf{0} \quad \mathbf{A} \quad \mathbf{0} \quad \mathbf{B}] \quad (3.111)$$

in which vectors $\mathbf{A}$ and $\mathbf{B}$ are established, respectively, as

$$\mathbf{A} = \|\mathbf{b}_{j,p}\|^2 \left(-\mathbf{b}_{j,p}^T \tilde{\mathbf{a}}_i + \mathbf{a}_i^T \left(\mathbf{s}_i \mathbf{b}_j^T \tilde{\mathbf{s}}_i + \mathbf{b}_j^T \mathbf{s}_i \tilde{\mathbf{s}}_i \right) \right) - \left(\mathbf{a}_i^T \mathbf{b}_{j,p} \right) \left(\mathbf{b}_{j,p}^T \left(\mathbf{s}_i \mathbf{b}_j^T \tilde{\mathbf{s}}_i + \mathbf{b}_j^T \mathbf{s}_i \tilde{\mathbf{s}}_i \right) \right) \quad (3.112)$$

$$\mathbf{B} = \|\mathbf{b}_{j,p}\|^2 \left(\mathbf{a}_i^T \left(-\tilde{\mathbf{b}}_j + \mathbf{s}_i \mathbf{s}_i^T \tilde{\mathbf{b}}_j \right) \right) - \left(\mathbf{a}_i^T \mathbf{b}_{j,p} \right) \left(\mathbf{b}_{j,p}^T \left(-\tilde{\mathbf{b}}_j + \mathbf{s}_i \mathbf{s}_i^T \tilde{\mathbf{b}}_j \right) \right) \quad (3.113)$$

and the right-hand side vector of the velocity constraint equations is as

$$\mathbf{v}^{(\phi,1)} = -\frac{\partial \Phi^{(\phi,1)}}{\partial t} = -\sin \phi^*(t) \dot{\phi}^*(t) \quad (3.114)$$

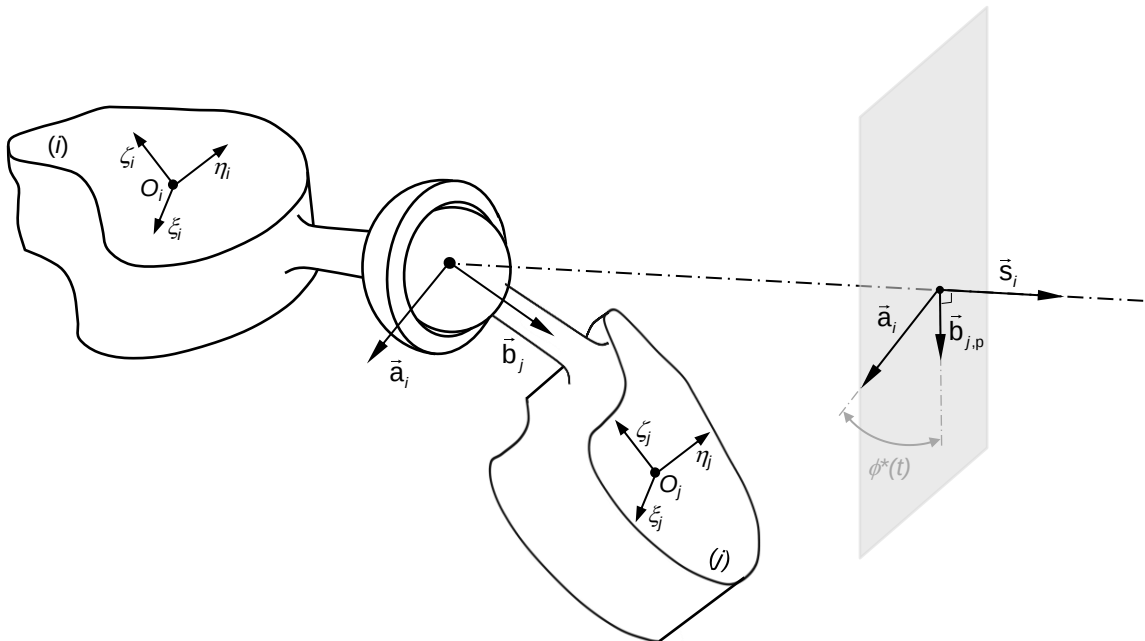


Figure 3.23 – Schematic representation of a spherical joint with vectors $\mathbf{a}_i$, $\mathbf{b}_j$, $\mathbf{b}_{j,p}$ and $\mathbf{s}_i$. The angle $\phi^*(t)$ is prescribed using experimental data.

The time derivative of Eq. (3.108) yields the acceleration constraint equation of the driving constraint (3.103) as

$$\ddot{\phi}^{(\phi,1)} \equiv \frac{1}{\|\mathbf{b}_{j,p}\|^6} \left(\|\mathbf{b}_{j,p}\|^3 \mathbf{C} - 3\|\mathbf{b}_{j,p}\|^2 \|\dot{\mathbf{b}}_{j,p}\| \left(\|\mathbf{b}_{j,p}\|^2 (\mathbf{b}_{j,p}^T \dot{\mathbf{a}}_i + \mathbf{a}_i^T \dot{\mathbf{b}}_{j,p}) - (\mathbf{a}_i^T \mathbf{b}_{j,p}) (\mathbf{b}_{j,p}^T \dot{\mathbf{b}}_{j,p}) \right) \right) + \cos \phi^*(t) \dot{\phi}^*(t)^2 + \sin \phi^*(t) \ddot{\phi}^*(t) = 0 \quad (3.115)$$

where vector $\mathbf{C}$ and the second time derivative of vector $\mathbf{b}_{j,p}$ are established, respectively, as

$$\begin{aligned} \mathbf{C} = & 2\|\mathbf{b}_{j,p}\| \|\dot{\mathbf{b}}_{j,p}\| (\mathbf{b}_{j,p}^T \dot{\mathbf{a}}_i + \mathbf{a}_i^T \dot{\mathbf{b}}_{j,p}) \\ & + \|\mathbf{b}_{j,p}\|^2 (\dot{\mathbf{a}}_i^T \dot{\mathbf{b}}_{j,p} + \mathbf{b}_{j,p}^T \ddot{\mathbf{a}}_i + \dot{\mathbf{b}}_{j,p}^T \dot{\mathbf{a}}_i + \mathbf{a}_i^T \ddot{\mathbf{b}}_{j,p}) \\ & - (\mathbf{b}_{j,p}^T \dot{\mathbf{a}}_i + \mathbf{a}_i^T \dot{\mathbf{b}}_{j,p}) (\mathbf{b}_{j,p}^T \dot{\mathbf{b}}_{j,p}) - (\mathbf{a}_i^T \mathbf{b}_{j,p}) (\dot{\mathbf{b}}_{j,p}^T \dot{\mathbf{b}}_{j,p} + \mathbf{b}_{j,p}^T \ddot{\mathbf{b}}_{j,p}) \end{aligned} \quad (3.116)$$

$$\ddot{\mathbf{b}}_{j,p} = \ddot{\mathbf{b}}_j - \dot{\mathbf{b}}_j^T \dot{\mathbf{s}}_i \mathbf{s}_i - \mathbf{s}_i^T \ddot{\mathbf{b}}_j \mathbf{s}_i - \dot{\mathbf{s}}_i^T \dot{\mathbf{b}}_j \dot{\mathbf{s}}_i - \dot{\mathbf{s}}_i^T \dot{\mathbf{b}}_j \mathbf{s}_i - \mathbf{b}_j^T \ddot{\mathbf{s}}_i \mathbf{s}_i - \mathbf{b}_j^T \dot{\mathbf{s}}_i \dot{\mathbf{s}}_i - \mathbf{s}_i^T \dot{\mathbf{b}}_j \dot{\mathbf{s}}_i - \mathbf{b}_j^T \dot{\mathbf{s}}_i \dot{\mathbf{s}}_i - \mathbf{b}_j^T \mathbf{s}_i \ddot{\mathbf{s}}_i \quad (3.117)$$

Taking into consideration the condition expressed in Eq. (3.31), then Eq. (3.115) becomes

$$\ddot{\phi}^{(\phi,1)} \equiv \frac{1}{\|\mathbf{b}_{j,p}\|^6} \left(\|\mathbf{b}_{j,p}\|^3 \mathbf{E} - 3\|\mathbf{b}_{j,p}\|^2 \|\dot{\mathbf{b}}_{j,p}\| \left(\|\mathbf{b}_{j,p}\|^2 (\mathbf{b}_{j,p}^T \dot{\mathbf{a}}_i + \mathbf{a}_i^T \dot{\mathbf{b}}_{j,p}) - (\mathbf{a}_i^T \mathbf{b}_{j,p}) (\mathbf{b}_{j,p}^T \dot{\mathbf{b}}_{j,p}) \right) \right) + \cos \phi^*(t) \dot{\phi}^*(t)^2 + \sin \phi^*(t) \ddot{\phi}^*(t) = 0 \quad (3.118)$$

in which vector $\mathbf{E}$ is expressed as

$$\begin{aligned} \mathbf{E} = & 2\|\mathbf{b}_{j,p}\| \|\dot{\mathbf{b}}_{j,p}\| (\mathbf{b}_{j,p}^T \dot{\mathbf{a}}_i + \mathbf{a}_i^T \dot{\mathbf{b}}_{j,p}) \\ & + \|\mathbf{b}_{j,p}\|^2 (\dot{\mathbf{a}}_i^T \dot{\mathbf{b}}_{j,p} + \mathbf{b}_{j,p}^T (-\tilde{\mathbf{a}}_i \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{a}}_i) + \dot{\mathbf{b}}_{j,p}^T \dot{\mathbf{a}}_i + \mathbf{a}_i^T \ddot{\mathbf{b}}_{j,p}) \\ & - (\mathbf{b}_{j,p}^T \dot{\mathbf{a}}_i + \mathbf{a}_i^T \dot{\mathbf{b}}_{j,p}) (\mathbf{b}_{j,p}^T \dot{\mathbf{b}}_{j,p}) - (\mathbf{a}_i^T \mathbf{b}_{j,p}) (\dot{\mathbf{b}}_{j,p}^T \dot{\mathbf{b}}_{j,p} + \mathbf{b}_{j,p}^T \ddot{\mathbf{b}}_{j,p}) \end{aligned} \quad (3.119)$$

and the second time derivative of vector $\mathbf{b}_{j,p}$ explicitly formulated in terms of the angular velocities of bodies i and j using Eq. (3.31) is established as

$$\begin{aligned} \ddot{\mathbf{b}}_{j,p} = & (-\tilde{\mathbf{b}}_j \dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{b}}_j) - \dot{\mathbf{b}}_j^T \dot{\mathbf{s}}_i \mathbf{s}_i - \mathbf{s}_i^T (-\tilde{\mathbf{b}}_j \dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{b}}_j) \mathbf{s}_i - \mathbf{s}_i^T \dot{\mathbf{b}}_j \dot{\mathbf{s}}_i - \dot{\mathbf{s}}_i^T \dot{\mathbf{b}}_j \mathbf{s}_i \\ & - \mathbf{b}_j^T (-\tilde{\mathbf{s}}_i \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i) \mathbf{s}_i - \mathbf{b}_j^T \dot{\mathbf{s}}_i \dot{\mathbf{s}}_i - \mathbf{s}_i^T \dot{\mathbf{b}}_j \dot{\mathbf{s}}_i - \mathbf{b}_j^T \dot{\mathbf{s}}_i \dot{\mathbf{s}}_i - \mathbf{b}_j^T \mathbf{s}_i (-\tilde{\mathbf{s}}_i \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i) \end{aligned} \quad (3.120)$$

Hence, the contribution to the right-hand side of the acceleration equations for the last driving constraint can be established as

$$\gamma^{(\phi,1)} = -\frac{1}{\|\mathbf{b}_{j,p}\|^6} \left(\|\mathbf{b}_{j,p}\|^3 \mathbf{F} - 3\|\mathbf{b}_{j,p}\|^2 \|\dot{\mathbf{b}}_{j,p}\| \left(\|\mathbf{b}_{j,p}\|^2 (\mathbf{b}_{j,p}^T \dot{\mathbf{a}}_i + \mathbf{a}_i^T \dot{\mathbf{b}}_{j,p}) - (\mathbf{a}_i^T \mathbf{b}_{j,p}) (\mathbf{b}_{j,p}^T \dot{\mathbf{b}}_{j,p}) \right) \right) - \cos \phi^*(t) \dot{\phi}^*(t)^2 - \sin \phi^*(t) \ddot{\phi}^*(t) \quad (3.121)$$

where vector $\mathbf{F}$ is defined as

$$\begin{aligned}\mathbf{F} = & 2\|\mathbf{b}_{j,p}\|\|\dot{\mathbf{b}}_{j,p}\|\left(\mathbf{b}_{j,p}^T\dot{\mathbf{a}}_i + \mathbf{a}_i^T\dot{\mathbf{b}}_{j,p}\right) \\ & + \|\mathbf{b}_{j,p}\|^2\left(\dot{\mathbf{a}}_i^T\dot{\mathbf{b}}_{j,p} + \mathbf{b}_{j,p}^T\ddot{\omega}_i\dot{\mathbf{a}}_i + \dot{\mathbf{b}}_{j,p}^T\dot{\mathbf{a}}_i + \mathbf{a}_i^T\mathbf{H}\right) \\ & - \left(\mathbf{b}_{j,p}^T\dot{\mathbf{a}}_i + \mathbf{a}_i^T\dot{\mathbf{b}}_{j,p}\right)\left(\mathbf{b}_{j,p}^T\dot{\mathbf{b}}_{j,p}\right) - \left(\mathbf{a}_i^T\mathbf{b}_{j,p}\right)\left(\dot{\mathbf{b}}_{j,p}^T\dot{\mathbf{b}}_{j,p} + \mathbf{b}_{j,p}^T\mathbf{H}\right)\end{aligned}\quad (3.122)$$

and vector $\mathbf{H}$ expresses the following

$$\begin{aligned}\mathbf{H} = & \ddot{\omega}_j\dot{\mathbf{b}}_j - \dot{\mathbf{b}}_j^T\dot{\mathbf{s}}_i\dot{\mathbf{s}}_i - \mathbf{s}_i^T\ddot{\omega}_j\dot{\mathbf{b}}_j\mathbf{s}_i - \mathbf{s}_i^T\dot{\mathbf{b}}_j\dot{\mathbf{s}}_i - \dot{\mathbf{s}}_i^T\dot{\mathbf{b}}_j\mathbf{s}_i \\ & - \mathbf{b}_j^T\ddot{\omega}_i\dot{\mathbf{s}}_i - \mathbf{b}_j^T\dot{\mathbf{s}}_i\dot{\mathbf{s}}_i - \mathbf{s}_i^T\dot{\mathbf{b}}_j\dot{\mathbf{s}}_i - \mathbf{b}_j^T\dot{\mathbf{s}}_i\dot{\mathbf{s}}_i - \mathbf{b}_j^T\dot{\mathbf{s}}_i\ddot{\omega}_i\dot{\mathbf{s}}_i\end{aligned}\quad (3.123)$$

3.5. Application Examples

Three examples are studied with the purpose of demonstrating the application of the approaches proposed in the previous sections to specific cases of biomechanics of motion. The first example presents a biomechanical model of the human leg and foot, and compares the kinematic outcomes of using either a modified or a classical universal joint for the ankle joint complex. The second example uses the same biomechanical model and shows the applicability of the RoM methodology to the ankle joint complex modeled as a modified universal joint only. The third example expands the second one to incorporate the thigh and pelvis, and demonstrate the application of the driving constraints formulation to human gait.

3.5.1. Application Example 1: Leg-Foot Model with Different Kinematic Joint Models for the Ankle Complex

A three-dimensional biomechanical multibody model implemented in a MATLAB in-house code named MUBODYNA (MULTiBODy DYNAMics) (Flores, 2012) is considered to compare the use of two kinematic joint models for the ankle complex of the human foot, namely a classical and a modified universal joint. The formulation for the classical universal joint can be consulted in P. Nikravesh (1988) and M. R. Silva et al. (2024a). The main difference between a classical and a modified universal joint is that the axes of the former intersect a given point P , while in the latter the joint axes are non-coplanar.

The developed biomechanical model is composed of three rigid bodies, namely the toes, the main foot, and the leg. Anatomically, the leg represents the tibia and fibula, the main foot is constituted by the tarsus and metatarsus, and the toes encompass the phalanges. The bodies of the biomechanical model are kinematically connected to each other by means of one revolute joint, connecting the toes to the main foot and representing the metatarsophalangeal articulations, and one universal joint, either classical or modified, connecting the main foot to the leg and representing the ankle joint complex. The translational and rotational

degrees-of-freedom of the leg are constrained. In addition, a constant angle kinematic constraint, similar to Eq. (3.22), is utilized on the metatarsophalangeal joint to lock the joint's angle. This procedure was performed in order to focus the analysis of the results exclusively on the differences between the two joint models considered for the ankle joint complex. The biomechanical multibody model has three degrees-of-freedom, but, since the metatarsophalangeal joint is subjected to a constant angle kinematic constraint, in reality, the model has two functional degrees-of-freedom only, arising from the universal joint. The two degrees-of-freedom represent the inversion/eversion and the plantarflexion/dorsiflexion of the main foot. The numbers of each body and their corresponding local coordinate systems are shown in Figure 3.24.

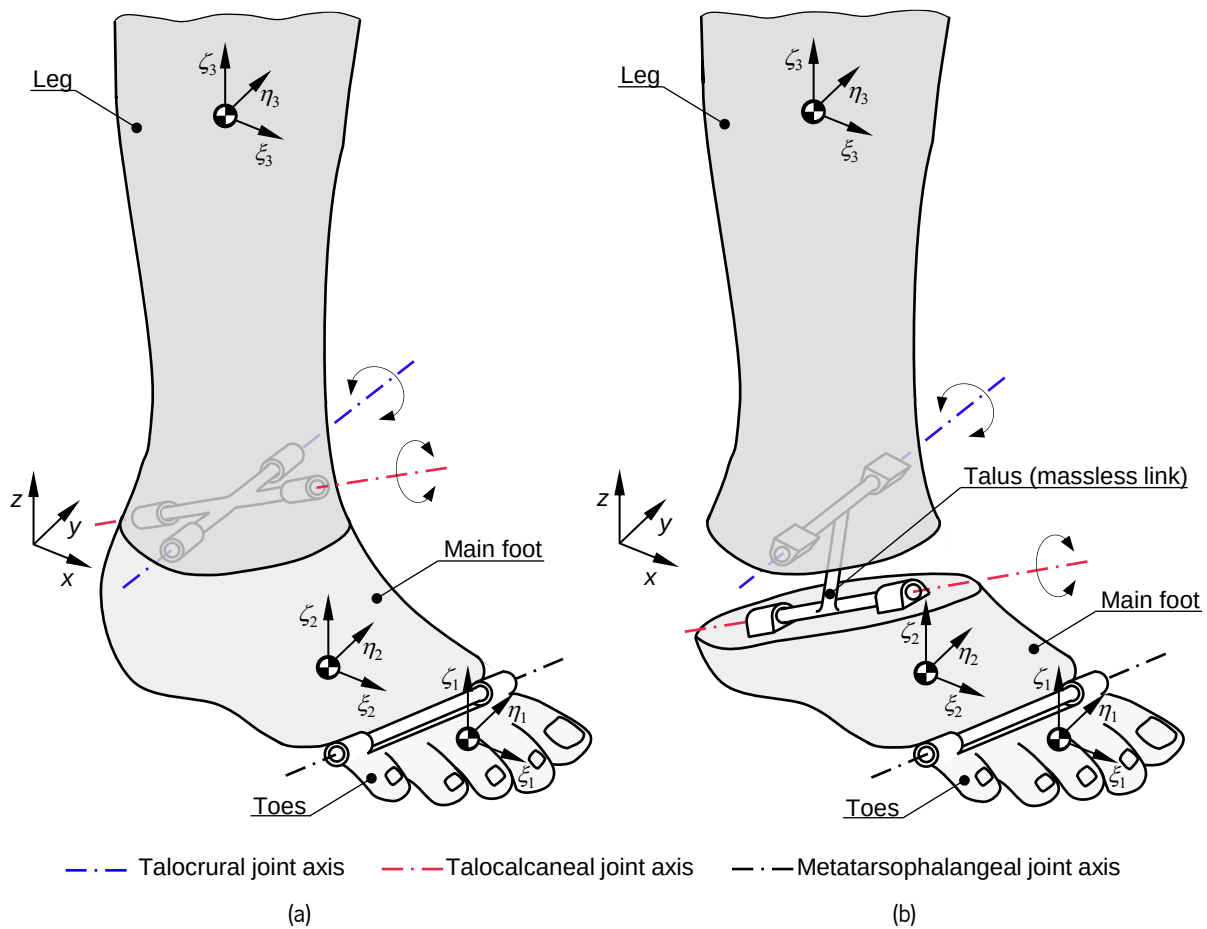


Figure 3.24 – Schematic representation of the biomechanical multibody model of the human leg, main foot, and toes with the ankle joint complex modeled as a (a) classical and (b) modified universal joint. The bodies are represented in different colors.

The generic configuration of the biomechanical model, where the numbers of each body and their corresponding local coordinate systems are shown, is displayed in Figure 3.24 and the corresponding initial conditions are listed in Table 3.1. The locations of all joints and the center of mass of all segments are assumed to be aligned with the midline of the foot, therefore resulting in a null y -coordinate. The $x, y,$ and z directions correspond to the anteroposterior, mediolateral and superoinferior directions in the three cardinal planes, respectively. For both biomechanical models presented in Figure 3.24, the location of

the talocrural joint is the same, as well as the orientation of its axis. In addition, the talocalcaneal joint axis has the same orientation on both models. The main difference between the models presented in Figure 3.24 is the location of the talocalcaneal joint. The model is released from the initial configuration with null velocities and under the action of the gravitational force, which acts on the negative z-direction.

Table 3.1 – Initial conditions for the biomechanical multibody model

Body (nr.)	x [m]	y [m]	z [m]	e_0	e_1	e_2	e_3
Toes (1)	0.2177	0.0000	0.0367	1.0000	0.0000	0.0000	0.0000
Main Foot (2)	0.0907	0.0000	0.0562	1.0000	0.0000	0.0000	0.0000
Leg (3)	0.0544	0.0000	0.3513	1.0000	0.0000	0.0000	0.0000

The dimensions and inertial properties of each body of the biomechanical model are listed in Table 3.2. It is important to note that the local reference frames of the bodies are located at their center of mass (see Figure 3.24) and are aligned with the principal axes of inertia. The model corresponds to a 71 kg and 1.77 m male subject (F. Anderson & Pandey, 1999). The total foot length is considered to be 0.27 m (F. Anderson & Pandey, 1999) and the length of the talus, which represents the length l_{m1} of the massless link, is taken as 0.0417 m (Siegler et al., 2014).

Table 3.2 – Dimensions and inertial properties of the bodies of the biomechanical multibody model

Body (nr.)	Length [m]	Mass [kg]	Moment of inertia [kg.m ²]		
			$I_{\xi\xi}$	$I_{\eta\eta}$	$I_{\zeta\zeta}$
Toes (1)	0.0797	0.2051	0.0001003	0.0001003	0.0002006
Main Foot (2)	0.1903	1.2000	0.0013818	0.0038337	0.0037110
Leg (3)	0.4300	3.5100	0.0477209	0.0483791	0.0048000

The location of the metatarsophalangeal, talocalcaneal and talocrural joints with respect to the local reference frames of the toes, main foot and leg can be consulted in Table 3.3.

Table 3.3 – Location of the joints of the biomechanical multibody model in local coordinates (F. Anderson & Pandey, 1999)

Joint	Body (nr.)	ξ [m]	η [m]	ζ [m]
Metatarsophalangeal	Toes (1)	-0.0274	0.0000	-0.0185
Metatarsophalangeal	Main Foot (2)	0.0996	0.0000	-0.0380
Talocalcaneal	Main Foot (2)	-0.0363	0.0000	0.0096
Talocalcaneal	Leg (3)	-0.0363	0.0000	0.0513
Talocrural	Leg (3)	0.0000	0.0000	-0.2438

The simulation parameters utilized in all dynamic simulations and in the numerical methods required to solve the dynamics of the system are displayed in Table 3.4.

Table 3.4 – Parameters used in the dynamic simulation of the biomechanical multibody model

Baumgarte coefficient - α	5	Reporting time step	0.00001 s
Baumgarte coefficient - β	5	Integration tolerance	10^{-10}
Integration algorithm	ode15s	Simulation time	5 s

The trajectory of the center of mass of the main foot in the sagittal (xz plane), transverse (xy plane), and frontal (yz plane) planes is represented in the plots of Figure 3.25. From the analysis of Figure 3.25a, it can be concluded that there are no substantial differences in the type and amplitude of motion performed by the two ankle joint models in the sagittal plane. This outcome is expected because the talocrural joint, which is the joint primarily responsible for the movement of the ankle in the sagittal plane, has the same location and its joint axis has the same orientation on both models. In turn, as already mentioned, although the talocalcaneal joint has the same orientation on both joint models, its location differs. Thus, in the transverse (Figure 3.25b) and frontal (Figure 3.25c) planes, the observed differences in the trajectory of the center of mass of the main foot are considerable in terms of amplitude and direction of movement. It should be noted that the amplitude of movement in the mediolateral direction (y -direction) allowed by the modified universal joint is greater than that allowed by the classical universal joint, which is observed by the fact that the red plot is wider than the blue plot in Figure 3.25b and Figure 3.25c. In addition, it can be noticed that the foot tends to move towards the lateral direction (negative y) when the classical universal joint is considered, as opposed to the case with the modified universal joint, in which the foot tends to move towards the medial direction (positive y). In order to better understand these differences in the mediolateral direction, it is important to recall that the main distinction between the two joint models for the ankle complex is the location of the talocalcaneal joint. In the classical universal joint, the talocrural and the talocalcaneal joints are coincident at point P , which corresponds to the anatomical location of the talocrural articulation. In modified universal joint, the two joint axes are non-coplanar due to the consideration of the massless link, which represents the talus bone. Thus, in this case, the talocalcaneal joint is closer to the center of mass of the main foot than when using the classical universal joint. The fact that the center of mass of the main foot is displaced from the location of the talocalcaneal joint in both joint models, generates a moment of force. The magnitude of this moment is smaller in the modified universal joint than in the classical universal joint, because the lever arm is also smaller. As a consequence, the amplitude of motion allowed by the modified universal joint in the mediolateral direction is greater than that observed for the classical universal joint. The incorporation of the massless link explains the differences between the two ankle joint models.

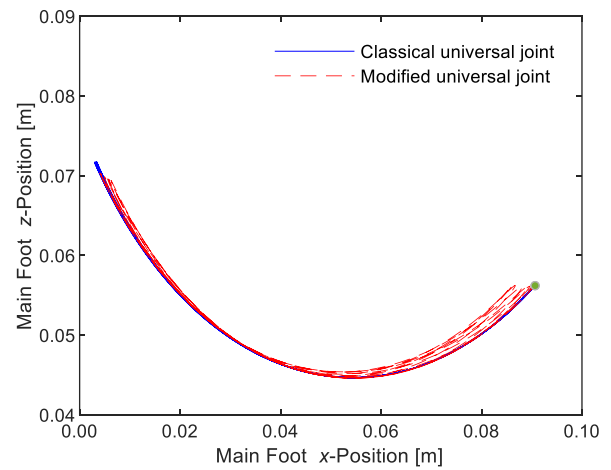
Classical universal joint



Modified universal joint



Sagittal plane

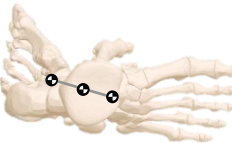


(a)

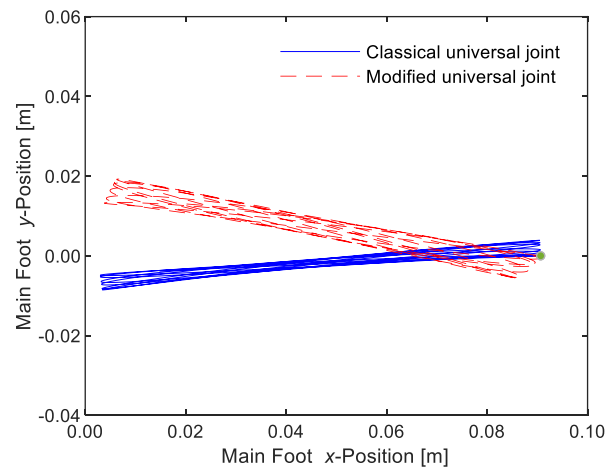
Classical universal joint



Modified universal joint



Transverse plane



(b)

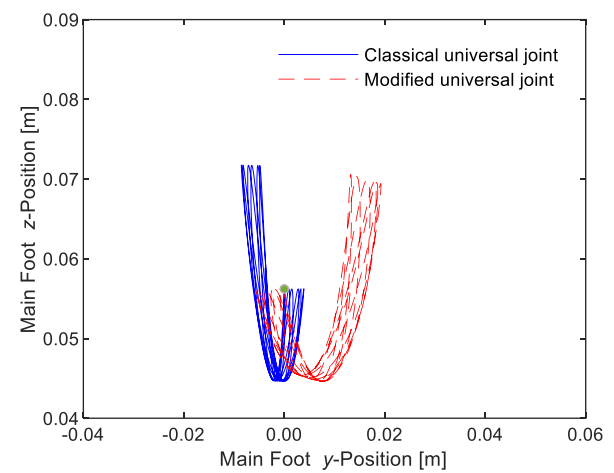
Classical universal joint



Modified universal joint



Frontal plane



(c)

Figure 3.25 – Trajectory of the center of mass of the main foot allowed by the two joint models considered to model the ankle joint complex of the human foot in the (a) sagittal, (b) transverse and (c) frontal planes. The green marker represents the initial position of the center of mass of the main foot. The x , y , and z directions correspond to the anteroposterior, mediolateral and superoinferior directions in the three cardinal planes, respectively.

To sum up, a comparison of the amplitude and type of movement allowed by the two kinematic joint models considered for the ankle joint complex of the human foot investigated in this application example is shown in the snapshots of Figure 3.26.

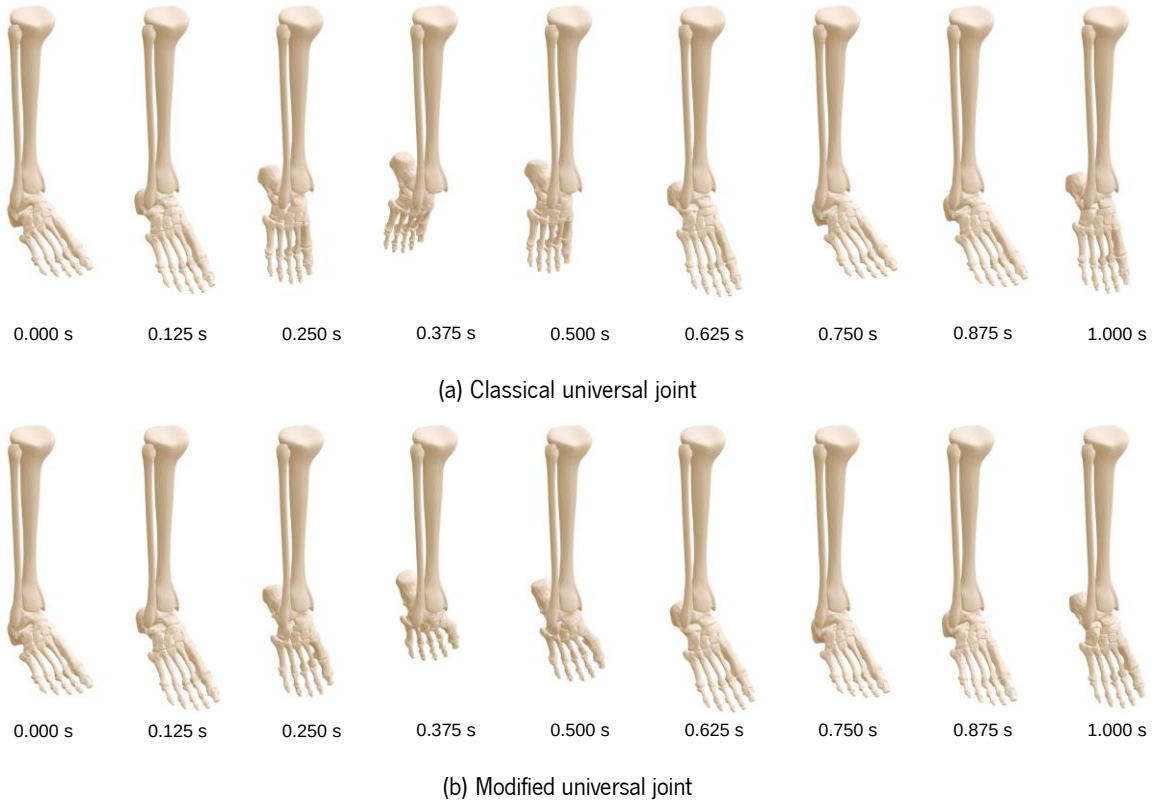


Figure 3.26 – Snapshots of the movement of the biomechanical multibody model for the first second of simulation using (a) the classical universal joint and (b) the modified universal joint. The model is subjected to the gravitational action only.

The time evolution of the velocity and acceleration of the center of mass of the main foot, as well as the phase portraits for the two ankle joint models are provided in Appendix A.

A second analysis is carried out, which aims at determining the influence of the massless link length (variable l_{ml} on Eq. (3.25)) on the response of the biomechanical multibody model. According to the study performed by Siegler et al. (2014), which utilized computational tomography data of 26 healthy subjects aged between 18 and 35 years old to quantify the three-dimensional morphology of the talus, the length of this bone was found to be 0.0417 ± 0.0057 m. Hence, in this study, four values for massless link length are tested, namely (i) 0.0000 m, which corresponds to the case of using the classical universal joint, (ii) 0.0360 m ($0.0417 - 0.0057$ m), (iii) 0.0417 m, and (iv) 0.0474 m ($0.0417 + 0.0057$ m). The second, third and fourth values are all considered in this study by utilizing a modified universal joint. In this analysis, the location of the talocrural joint was not altered, but the location of the talocalcaneal joint was adjusted to accommodate the previously mentioned variations on the massless link length. A schematic representation of the four cases is presented in Figure 3.27.

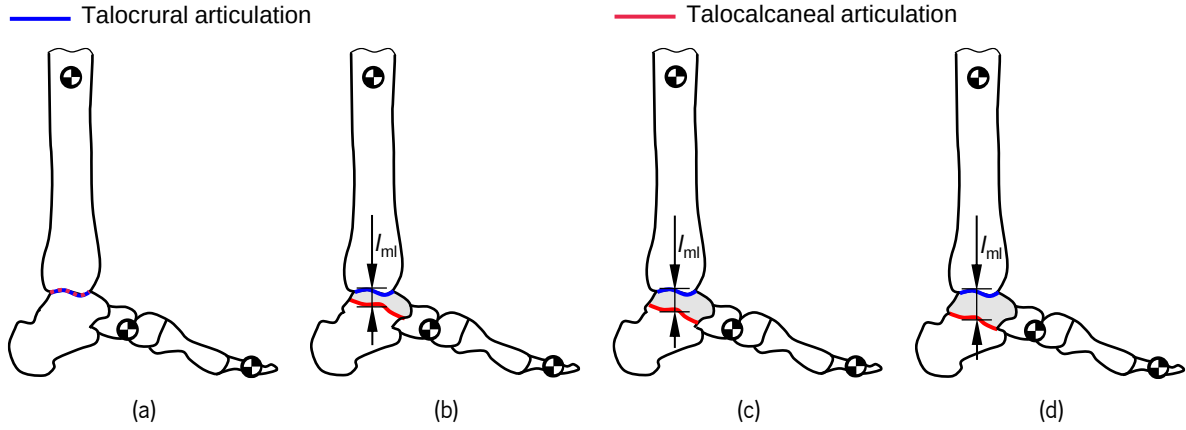


Figure 3.27 – Schematic representation, in the sagittal plane, of the cases tested for the massless link length, l_{ml} , specifically (a) 0.0000, (b) 0.0360, (c) 0.0417, and (d) 0.0474 m. The talus bone is highlighted in grey.

Based on Figure 3.25, it can be concluded that the use of the modified universal joint incorporated with the massless link to model the ankle joint complex of the human foot introduces substantial differences primarily on the mediolateral direction (y -direction). Thus, only the mediolateral direction is studied in this analysis, and the obtained results for the trajectory of the center of mass of the main foot are depicted in the plots of Figure 3.28. Observing Figure 3.28, it can be concluded that, as the length of the massless link increases, the center of mass of the main foot moves progressively to the medial direction (positive y) on the transverse and frontal planes. The most distinct plot is the one in which the massless link length is equal to 0.000 m, corresponding to the classical universal joint model. In addition, the amplitude of motion of the center of mass of the main foot increases with the increase in the massless link length, as concluded by the successive increase in the width of the plots. Having these conclusions in mind, it should be recognized that altering the massless link length strongly influences the response of the model, leading to different results.

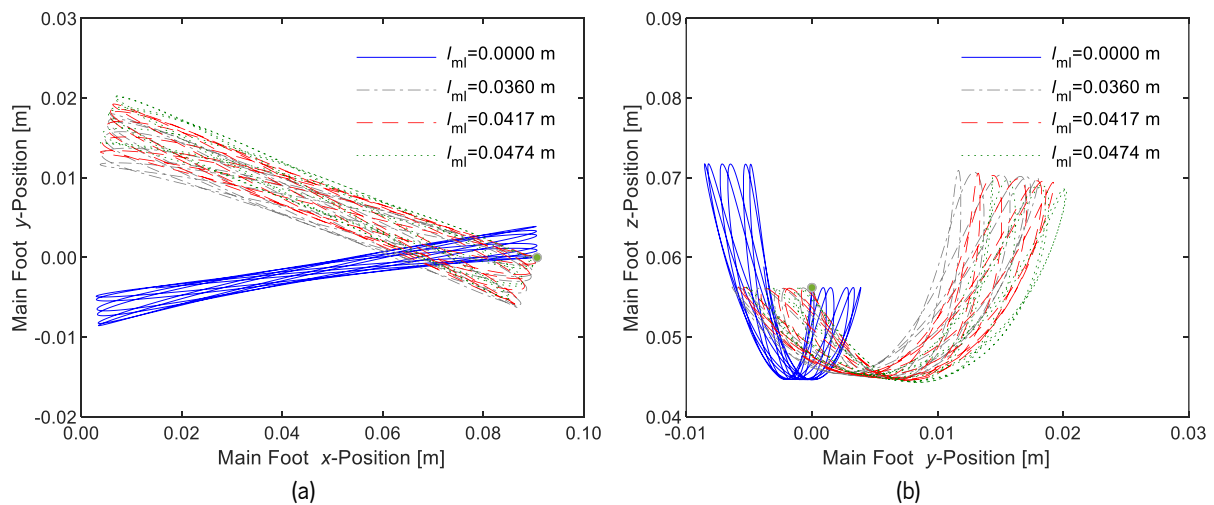


Figure 3.28 – Influence of the massless link length on the response of the biomechanical multibody model. Trajectory of the center of mass of the main foot in the (a) transverse and (b) frontal planes. The x , y , and z directions correspond to the anteroposterior, mediolateral and superoinferior directions in the three cardinal planes, respectively.

3.5.2. Application Example 2: Leg-Foot Model with Range of Motion Restriction

In this application example, the biomechanical multibody model presented in the first example is also considered. However, for the purpose of the present analysis, only the modified universal joint is utilized to model the ankle joint complex of the human foot. The aim of this application example is to demonstrate the potential of applying the methodology to restrict the RoM of joints presented in section 3.3 to the complex case of the human ankle joint. A detailed description is provided, which includes the definition of the local reference frames of the joint and corresponding circumduction cones, estimation of the longitude and latitude, calculation of the maximum latitude using the elliptical approach and the transfer of forces and moments to the adjacent bodies.

As previously mentioned, the metatarsophalangeal joint angle of the biomechanical model is locked using Eq. (3.22), and, thus, it is not necessary to restrict the corresponding RoM. In this sense, only the talocrural and talocalcaneal joints are subjected to the joint resistance moments of Eq. (3.34). For the application of the methodology, the modified universal joint can be thought of as two separate revolute joints, meaning that the RoM associated with each joint axis must be restricted independently.

As explained in section 3.3, the circumduction cone is characterized by defining the axes of the joint's local coordinate system using the local coordinate system of the reference body. For the talocrural and talocalcaneal joints, the reference bodies are the leg and the main foot, respectively. In the cones illustrated in Figure 3.29, the unit vectors defining the ξ_h , η_h and ζ_h axes are established as

$$\begin{aligned}\mathbf{u}'_{\xi,h} &= \{\cos \varepsilon \quad -\sin \varepsilon \quad 0\}^T \\ \mathbf{u}'_{\eta,h} &= \{-\sin \varepsilon \cos \tau_{re} \quad -\cos \varepsilon \cos \tau_{re} \quad -\sin \tau_{re}\}^T \\ \mathbf{u}'_{\zeta,h} &= \{\sin \varepsilon \sin \tau_{re} \quad \cos \varepsilon \sin \tau_{re} \quad -\cos \tau_{re}\}^T\end{aligned}$$

for the talocrural joint (see Figure 3.29a) and as

$$\begin{aligned}\mathbf{u}'_{\xi,h} &= \{\cos \rho \cos \theta_{re} \quad \sin \rho \cos \theta_{re} \quad \sin \theta_{re}\}^T \\ \mathbf{u}'_{\eta,h} &= \{-\sin \rho \quad \cos \rho \quad 0\}^T \\ \mathbf{u}'_{\zeta,h} &= \{-\cos \rho \sin \theta_{re} \quad -\sin \rho \sin \theta_{re} \quad \cos \theta_{re}\}^T\end{aligned}$$

for the talocalcaneal joint (see Figure 3.29b).

After the definition of the joint's local coordinate system, the unit vector, $\mathbf{u}_{i,h}$, which allows to identify, in every configuration, the orientation of the moving body in the joint's local coordinate system, with the exception of the internal rotation, must be established. For the talocrural and talocalcaneal joints,

the moving bodies are the main foot and the leg, respectively. In a modified universal joint, vector $\mathbf{u}_{r,h}$ is the massless link. However, in order to ensure that the RoM associated with each joint is correctly restricted, vector $\mathbf{u}_{r,h,p}$, which denotes the projection of the massless link onto the plane perpendicular to the axis of the joint which RoM is intended to be restricted, must be considered. Vector $\mathbf{u}_{r,h,p}$ is calculated using the following condition (see Figure 3.29 and Figure 3.30)

$$\mathbf{u}_{r,h,p} = \frac{\mathbf{u}_{r,h} - (\mathbf{u}_{r,h}^T \mathbf{s}_i) \mathbf{s}_i}{\|\mathbf{u}_{r,h} - (\mathbf{u}_{r,h}^T \mathbf{s}_i) \mathbf{s}_i\|} \quad (3.124)$$

where $\mathbf{u}_{r,h,p}$ is the projection of vector $\mathbf{u}_{r,h}$, and $\mathbf{s}_i$ represents a unit vector along the joint axis given either by Eqs. (3.17) or (3.18) (see Figure 3.30). Since the massless link does not belong to any particular body, vectors $\mathbf{u}_{r,h}$ and $\mathbf{u}_{r,h,p}$ do not have constant coordinates in any of the local coordinate systems.

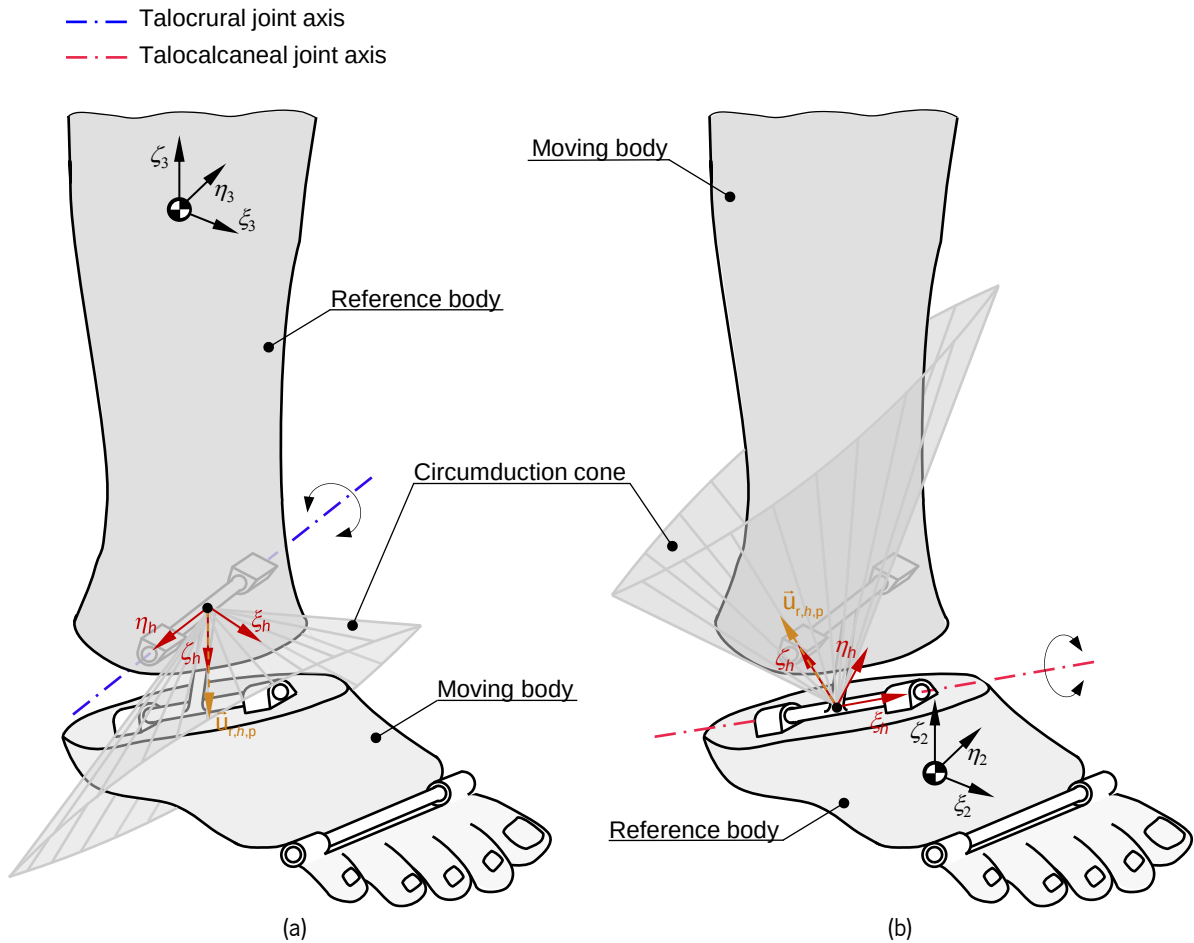


Figure 3.29 – Schematic representation of the circumduction cones for the (a) talocrural and (b) talocalcaneal joints.

Figure 3.30 provides a schematic representation of two bodies i and j connected by a modified universal joint, with joint axis $\mathbf{s}_i$ and $\mathbf{s}_j$, respectively. An example is given for the $\mathbf{s}_i$ joint axis. The massless link, vector $\mathbf{u}_{r,h}$, and the projection of the massless link onto the plane perpendicular to the $\mathbf{s}_i$ joint axis, vector $\mathbf{u}_{r,h,p}$, are illustrated.

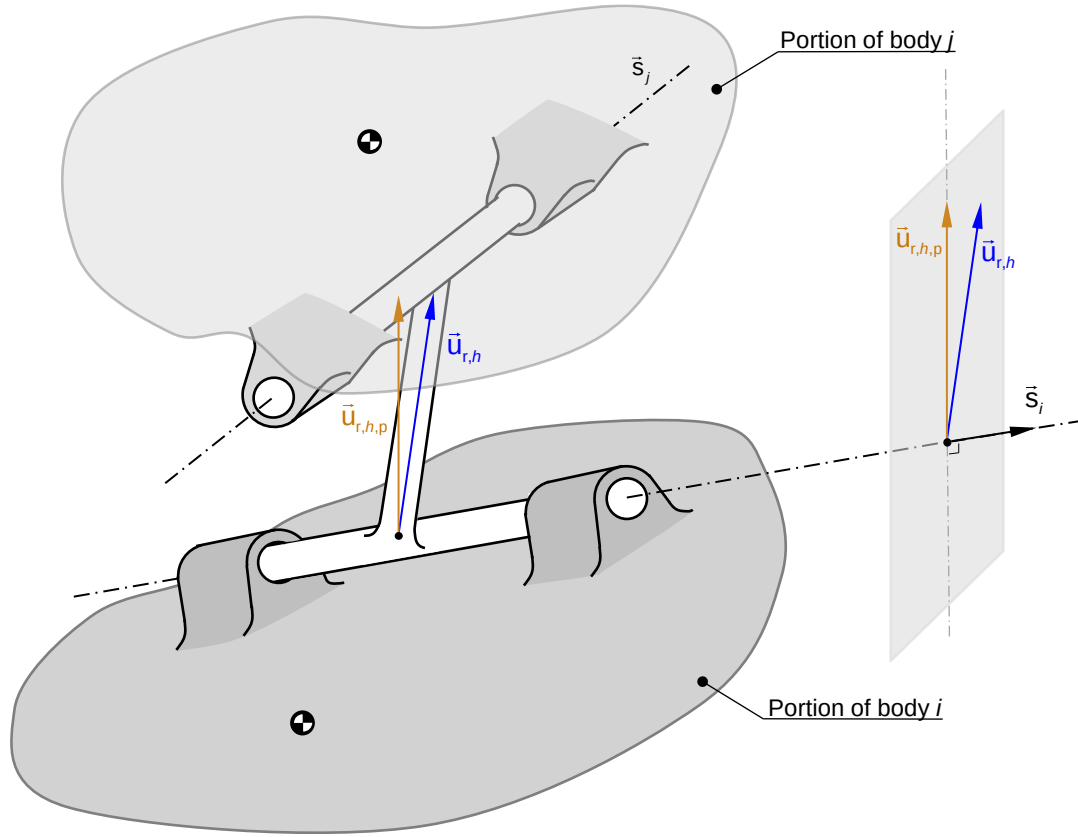


Figure 3.30 – Schematic representation of two bodies i and j connected by a modified universal joint, with joint axis s_i and s_j , respectively. Vectors $\mathbf{u}_{r,h}$ and $\mathbf{u}_{r,h,p}$ are illustrated.

In this work, the maximum latitude for talocrural dorsiflexion and plantarflexion is considered to be 20° and 35° , respectively. In turn, talocalcaneal maximum inversion and eversion are defined as 35° and 25° , respectively (Panero & Zelnik, 1979). Since, in a modified universal joint, the restriction of the RoM is achieved by considering two separate revolute joints, two circumduction cones must be constructed. The longitude is defined, for both joints, as

$$\Psi_h = \{0^\circ \quad 90^\circ \quad 180^\circ \quad 270^\circ \quad 360^\circ\}$$

and the maximum latitude for the talocrural and talocalcaneal joints is defined, respectively, as

$$\sigma_{h,\max} = \{20^\circ \quad 1^\circ \quad 35^\circ \quad 1^\circ \quad 20^\circ\} \quad \text{and} \quad \sigma_{h,\max} = \{1^\circ \quad 25^\circ \quad 1^\circ \quad 35^\circ \quad 1^\circ\}$$

The differences in the maximum latitude are associated with the definition of the joint's local coordinate system for each joint (see Figure 3.29). Furthermore, a value of 1° is utilized as a tolerance in the locations of the circumduction cone that are not reached by the moving body due to the kinematic structure of a revolute joint. As observed in the above conditions, the maximum allowable latitude for both the talocrural and talocalcaneal joints is defined for longitude values that coincide with the limits of the four main quadrants, namely 0° , 90° , 180° , 270° and 360° (see Figure 3.31). Thus, the maximum allowable latitude for any longitude must be calculated using the elliptical approach.

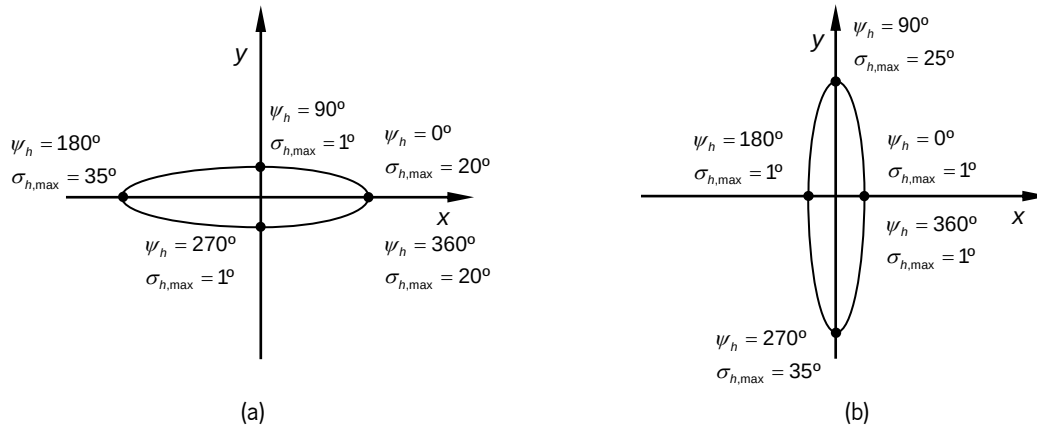


Figure 3.31 – Schematic representation of the top view of the circumduction cone with the longitude and maximum latitude specified for the (a) talocrural and (b) talocalcaneal joints.

It is important to recall that, in the following formulation, the reference and moving bodies are denoted as bodies i and j , respectively. When the moving body is located in an unacceptable configuration, the joint motion-restricting moment (3.63) is applied to the reference body, $\mathbf{m}_{h,i}^{\text{mr}}$, and to the massless link, $\mathbf{m}_{h,\text{ml}}^{\text{mr}}$. However, since the massless link is a vector connecting two bodies and it does not belong to any of them, the joint motion-restricting moment is not directly applied to the moving body. Thus, the moment applied to the massless link, $\mathbf{m}_{h,\text{ml}}^{\text{mr}}$, must be transferred to the moving and reference bodies. A representation of the force and moment transfer phenomenon is shown in Figure 3.32.

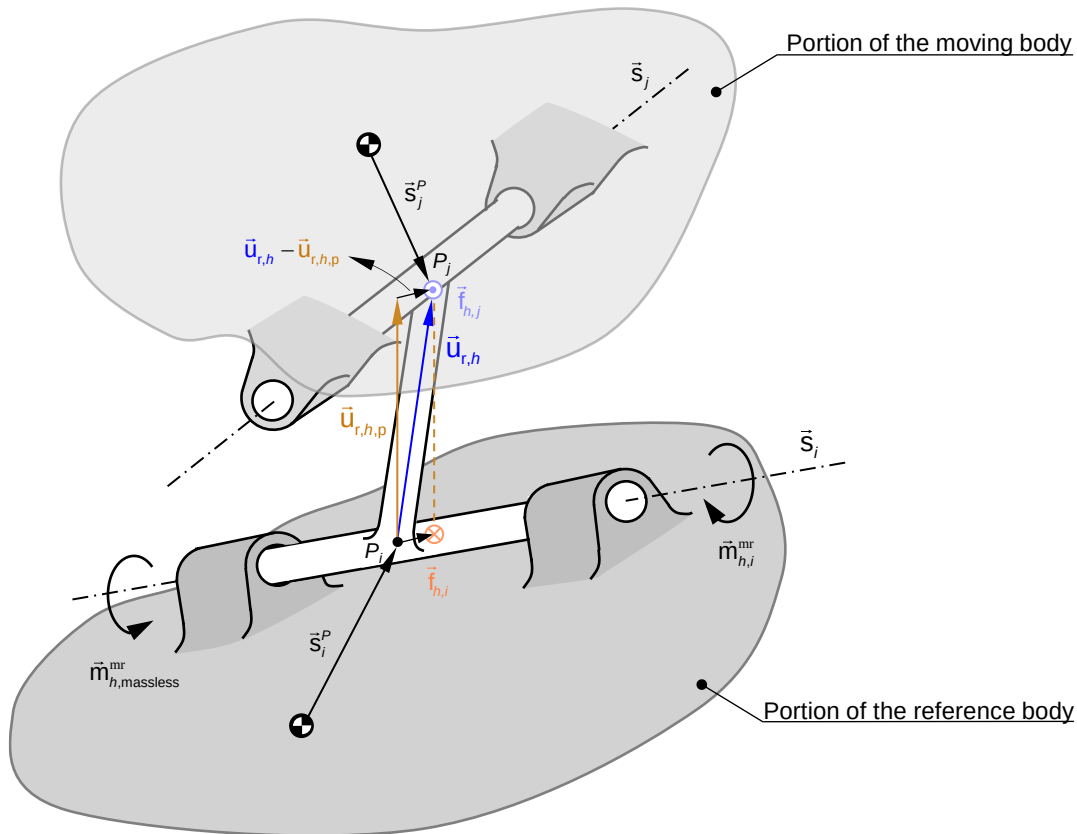


Figure 3.32 – Schematic representation of the force and moment transfer phenomenon in a modified universal joint.

The joint motion-restricting moment applied to the massless link, $\mathbf{m}_{h,ml}^{mr}$, generates a force on the reference body, $\mathbf{f}_{h,i}$, which is calculated as

$$\mathbf{f}_{h,i} = \left(\frac{\tilde{\mathbf{u}}_{r,h,p} \mathbf{m}_{h,ml}^{mr}}{\|\mathbf{u}_{r,h,p}\| \|\mathbf{m}_{h,ml}^{mr}\|} \right) f_{h,i} \quad (3.125)$$

where $f_{h,i}$ is the force magnitude evaluated as

$$f_{h,i} = \frac{\|\mathbf{m}_{h,ml}^{mr}\|}{\|\mathbf{u}_{r,h,p}\|} \quad (3.126)$$

Force $\mathbf{f}_{h,i}$ generates a moment on the reference body, which is established as

$$\mathbf{m}_{h,i} = \tilde{\mathbf{l}}_{h,i} \mathbf{f}_{h,i} \quad (3.127)$$

where $\mathbf{l}_{h,i}$ is the moment lever arm from the point of force application to the center of mass of the reference body, which, as shown in Figure 3.32, can be calculated as

$$\mathbf{l}_{h,i} = \mathbf{s}_i^P + (\mathbf{u}_{r,h} - \mathbf{u}_{r,h,p}) \quad (3.128)$$

The force applied to the reference body, $\mathbf{f}_{h,i}$, must be applied to the moving body with opposite direction, $\mathbf{f}_{h,j}$, as

$$\mathbf{f}_{h,j} = -\mathbf{f}_{h,i} \quad (3.129)$$

The force $\mathbf{f}_{h,j}$ produces a moment because its application point is displaced from the center of mass of the moving body as

$$\mathbf{m}_{h,j} = \tilde{\mathbf{s}}_j^P \mathbf{f}_{h,j} \quad (3.130)$$

Concerning the joint dissipative moment of Eq. (3.65), in this work, the damping coefficient for the ankle joint complex, j_h , is obtained by multiplying the total mass of the considered subject (71 kg) by the normalized value 0.008 N·m·s/kg (Rouse et al., 2014; Shorter & Rouse, 2018). Thus, a value of 0.5680 N·m·s is utilized. Since two circumduction cones are considered for the application of the RoM methodology, half of this value is applied to each cone (0.2840 N·m·s). Due to the existence of the massless link in a modified universal joint, the angular velocity of each joint is calculated based on the velocities of the adjacent bodies as (see Figure 3.33)

$$\begin{aligned} \boldsymbol{\omega}_h = & -\frac{1}{\|\mathbf{u}_{r,h,p}\| \sin \varphi} \left(\mathbf{a}_i^T (\mathbf{s}_i \mathbf{s}_i^T - \mathbf{I}) \dot{\mathbf{r}}_i + \left(-\mathbf{u}_{r,h,p}^T \tilde{\mathbf{a}}_i + \mathbf{a}_i^T (\tilde{\mathbf{s}}_i^P - \mathbf{s}_i \mathbf{s}_i^T \tilde{\mathbf{s}}_i^P + \mathbf{s}_i \mathbf{u}_{r,h}^T \tilde{\mathbf{s}}_i + \mathbf{u}_{r,h}^T \mathbf{s}_i \tilde{\mathbf{s}}_i) \right) \boldsymbol{\omega}_i \right. \\ & \left. + \mathbf{a}_i^T (\mathbf{I} - \mathbf{s}_i \mathbf{s}_i^T) \dot{\mathbf{r}}_j + \mathbf{a}_i^T (\mathbf{s}_i \mathbf{s}_i^T \tilde{\mathbf{s}}_j^P - \tilde{\mathbf{s}}_j^P) \boldsymbol{\omega}_j \right) \end{aligned} \quad (3.131)$$

in which $\mathbf{a}_i$ represents one arbitrary unit vector perpendicular to the $\mathbf{s}_i$ joint axis, φ is the joint angle, which is measured between vectors $\mathbf{a}_i$ and $\mathbf{u}_{r,h,p}$, as represented in Figure 3.33 for the case of the talocalcaneal joint, $\mathbf{s}_k^P$ ($k=i, j$) is the global position vector of point P located on body k with respect to the body's local coordinate system, $\mathbf{I}$ denotes the identity matrix, $\dot{\mathbf{r}}_k$ denotes the velocity vector of the center of mass of body k described in global coordinates, and $\boldsymbol{\omega}_k$ denotes the angular velocity vector of body k .

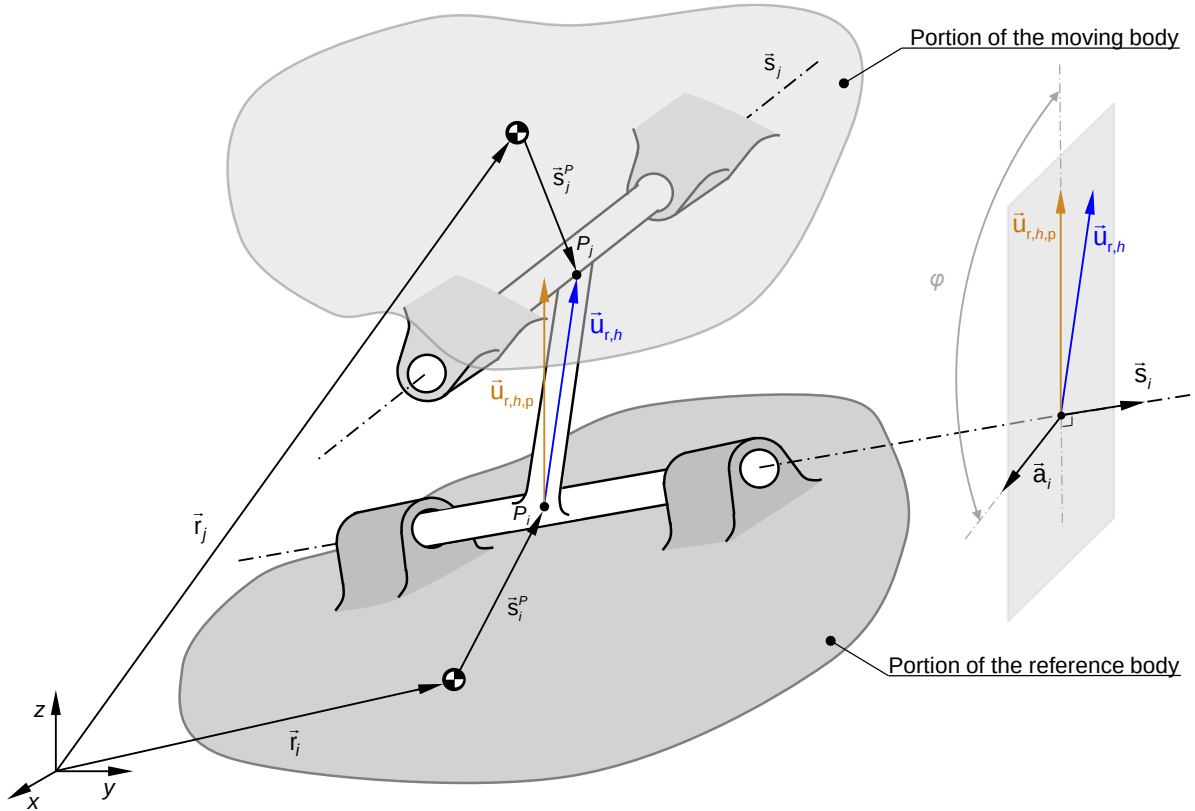
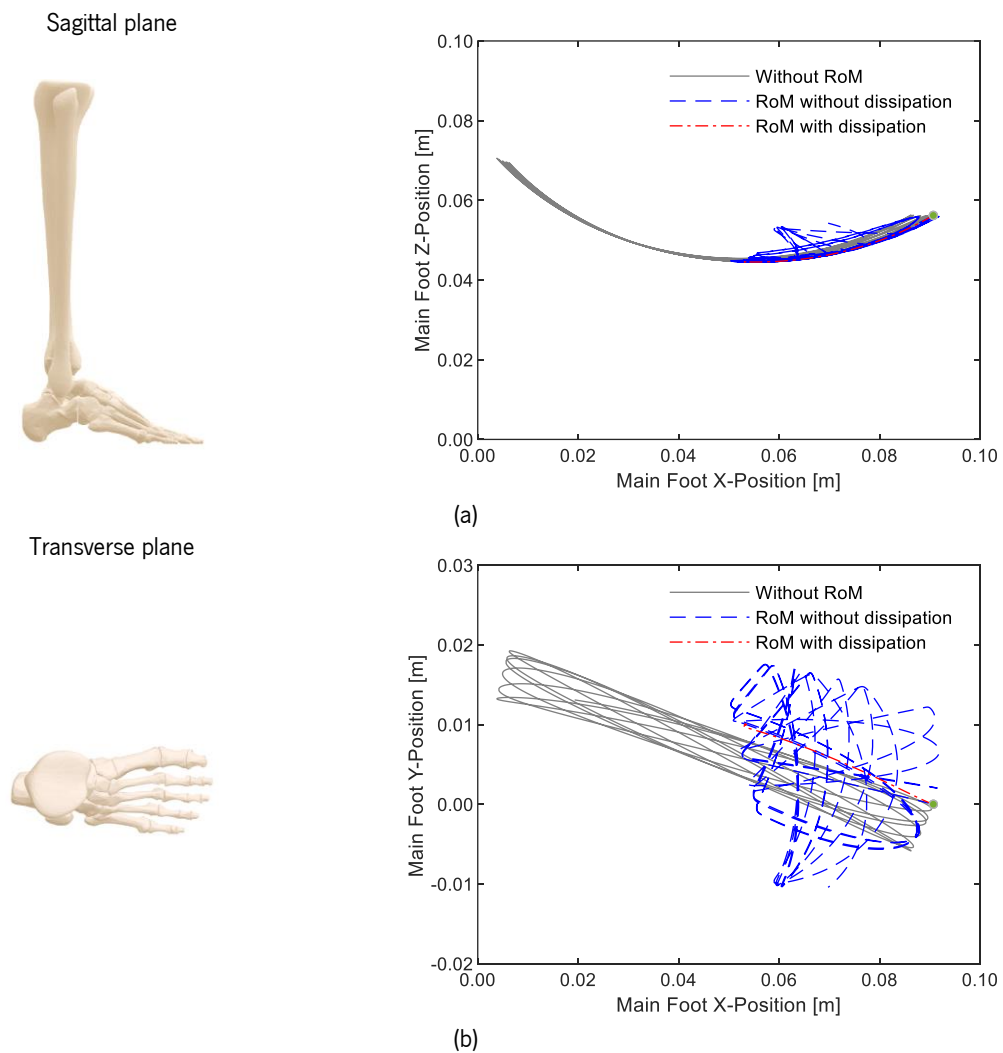


Figure 3.33 – Representation of the vectors utilized to calculate the angular velocity of each joint of a modified universal joint.

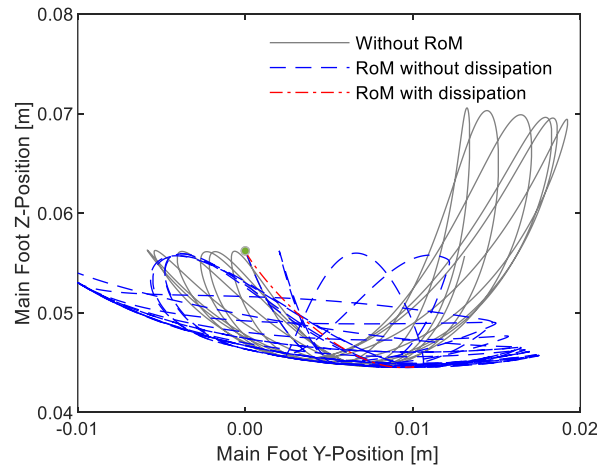
In what follows, the results of three analyses are shown. In the first analysis, the model is released from the initial position, with null velocities, and under the action of the gravitational force only. The second and third analyses are similar to the first case but include the joint resistance moments to restrict the RoM of the ankle joint complex without and with energy dissipation, respectively. For both joints, $\Delta\sigma_h$ and $m_{pe,h}$ are taken as 11.5° and $226 \text{ N}\cdot\text{m}$, respectively (M. P. T. Silva et al., 1996, 1997)

The trajectory of the center of mass of the main foot throughout the simulation in the three cardinal planes can be observed in Figure 3.34. The initial conditions defined for the biomechanical model, in which, in the initial configuration, the foot is horizontal with respect to the ground, prevent the talocrural joint from reaching its maximum latitude for dorsiflexion. For the talocalcaneal joint, no limitation is imposed by the initial conditions. Analyzing Figure 3.34, significant differences in the trajectory of the center of mass of the

main foot are observed for all analyses and cardinal planes. For talocrural plantarflexion, the amplitude of movement of the center of mass is higher when the RoM methodology is not considered. In turn, when the methodology is applied, with or without energy dissipation, the amplitude of movement is significantly decreased. This fact can be observed in the anteroposterior (x -direction) and superoinferior (z -direction) directions (see Figure 3.34). The maximum latitude for eversion is not reached for the talocalcaneal joint in the case where the methodology is not applied, as concluded by the fact that, in Figure 3.34b and Figure 3.34c, the blue plot reaches higher values than the grey plot in the lateral direction (negative y). For talocalcaneal inversion (medial direction, positive y), the model exceeds the maximum latitude in the first analysis, but this occurrence is corrected with application of the RoM methodology. For the case without energy dissipation, the trajectory of the center of mass of the main foot is less smooth due to the successive joint resistance moment applications to prevent the RoM from being exceeded, which impose successive changes of direction. With the addition of energy dissipation to the system, a smoother behavior on the trajectory of the center of mass of the main foot is observed in all cardinal planes.



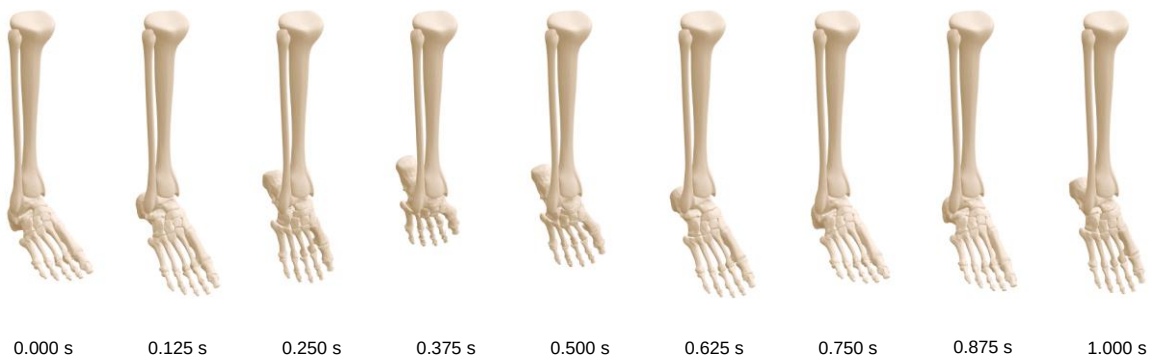
Frontal plane



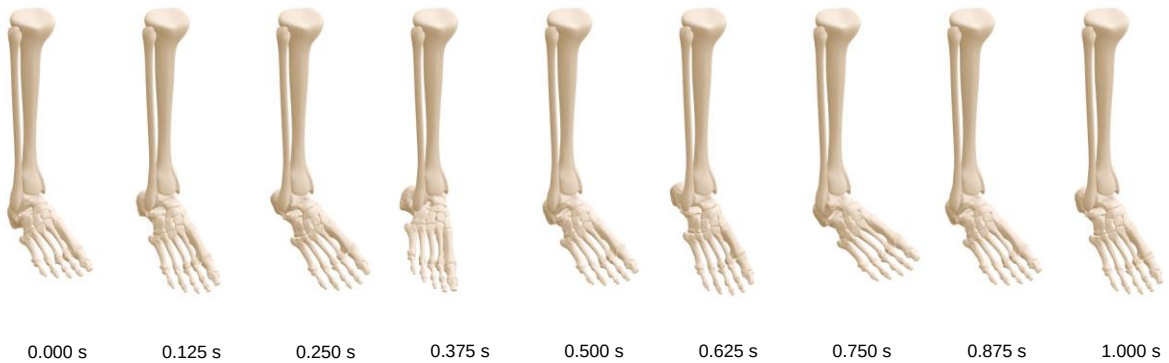
(c)

Figure 3.34 – Trajectory of the center of mass of the main foot in the (a) sagittal, (b) transverse and (c) frontal planes. The green marker represents the initial position of the center of mass of the main foot. The x , y , and z directions correspond to the anteroposterior, mediolateral and superoinferior directions in the three cardinal planes, respectively.

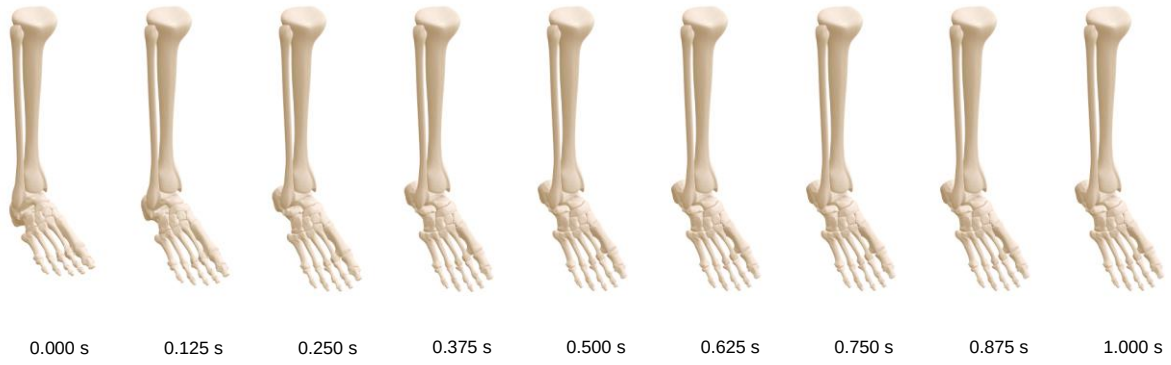
Figure 3.35 presents several snapshots of the movement of the biomechanical multibody model for the first second of simulation in order to provide a comparison of the amplitude and type of movement between the three tested cases in Figure 3.34.



(a) Gravitational action only



(b) RoM methodology without energy dissipation



(c) RoM methodology with energy dissipation

Figure 3.35 – Snapshots of the movement of the biomechanical model for the first second of simulation (a) subjected to gravitational action only, and with the RoM methodology (b) without and (c) with energy dissipation.

In order to examine whether the maximum latitude for plantarflexion, eversion and inversion is properly restricted with the application of the proposed RoM methodology, the evolution of the latitude as a function of the longitude for the talocrural and talocalcaneal joints is depicted in Figure 3.36.

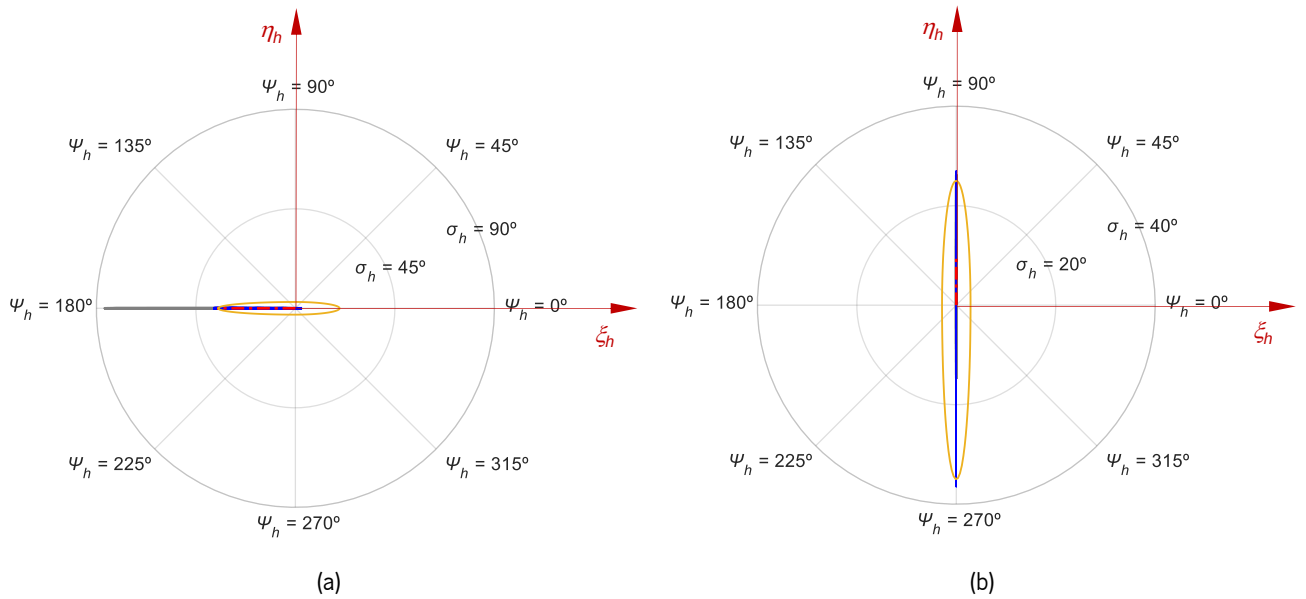


Figure 3.36 – Variation of the latitude as a function of the longitude for the (a) talocrural and (b) talocalcaneal joints. These figures represent the top view of the joint's local coordinate system: case without RoM (---), RoM without dissipation (—), RoM with dissipation (— · —), and limits of the circumduction cone (— · —).

When the RoM methodology is not considered, the model exceeded the maximum latitude for plantarflexion since a latitude of almost 90° is reached for $\psi_h = 180^\circ$ (see Figure 3.36a), as opposed to a maximum latitude of 37° and 35° observed when the RoM methodology is considered without and with energy dissipation, respectively (see Figure 3.36a and Figure 3.36c). When energy dissipation is not considered, the latitude exceeds the maximum allowable latitude by 2° because a value of 11.5° was set for parameter $\Delta\sigma_h$, which allows to adjust the joint stiffness. Thus, the RoM is not exceeded. Furthermore, the maximum latitude for dorsiflexion is not reached ($\psi_h = 0^\circ$). It must be emphasized that, in the present

application example, when the RoM methodology is taken into account with energy dissipation the model reaches the equilibrium position in the maximum latitude for plantarflexion, since the gravitational force tends to lead the foot outwards its normal RoM. For the talocalcaneal joint, as concluded previously in Figure 3.34, when the RoM is not considered, the maximum latitude for eversion is not reached ($\psi_h = 270^\circ$), as opposed to the maximum latitude for inversion ($\psi_h = 90^\circ$). In the cases in which the RoM methodology is applied, the maximum latitude for both of these movements is adequately restricted to the respective defined values, considering the parameter $\Delta\sigma_h$ (see Figure 3.36b and Figure 3.36d).

The evolution of the joint resistance moments for the talocrural and talocalcaneal joints through the simulation time, as well as the variation of the mechanical energy are presented in Appendix B.

Since the required calculations for the three compared scenarios do not differ significantly, the computational cost of the model was evaluated through the number of function evaluations, and it is depicted in Figure 3.37. When energy dissipation is considered and the 5-second simulation is utilized to evaluate the computational cost, the system shows numerical issues after it is fully dampened. These issues are directly associated with the numerical error that arises from the integration process and that does not allow to obtain exactly null velocities and, thus, fully stop the motion of the bodies. In turn, very low velocities are calculated using Eq. (3.14), which provoke variations in the position and velocity of the bodies, leading to a continuous application of a joint dissipative moment to the system. The dissipative moment provokes significant variations, in relative terms, of the coordinates of the model, which reduce the time step required to meet the specified tolerances and proceed with the integration process, significantly decreasing the computational efficiency. In order to ensure that this issue does not affect the analysis, Figure 3.37 shows the computational cost for 1 s of simulation, which represents the simulation time prior to the occurrence of the numerical issues. The most efficient case is the one in which the RoM methodology is not considered, while the case without energy dissipation is the least efficient one.

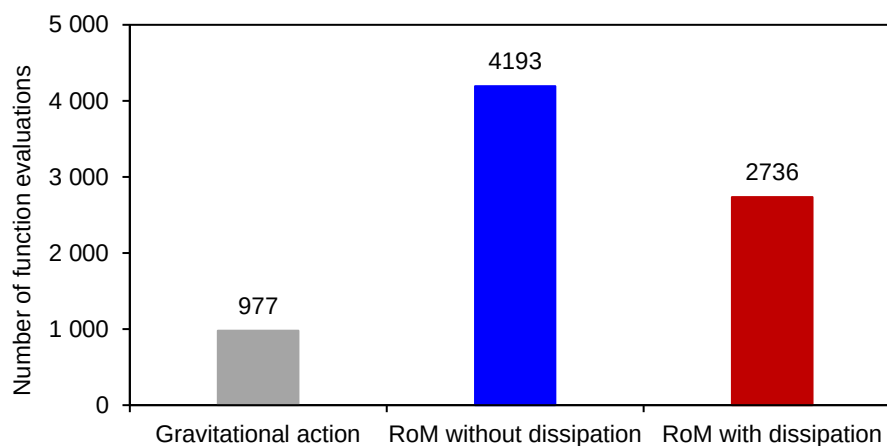


Figure 3.37 – Computational cost for the biomechanical multibody model for 1 second of simulation.

3.5.3. Application Example 3: Lower Limb Model with Driving Constraints

The aim of this application example is to demonstrate the potential of the driving constraints formulated in section 3.4 to guide the degree-of-freedom of a biomechanical multibody model. The use of the driving constraints requires the acquisition of experimental data of the human motion. This procedure is associated with other concepts not clarified in this work yet, including the description of the equipment utilized in the biomechanics laboratory, the definition of the market set protocol, and the explanation of the kinematic consistency and data treatment procedures. Hence, to the scope of this section, the previously mentioned concepts are not described here and are addressed in detail in Chapter 5. The anthropometric data, definition of the bodies' local coordinate systems and location of the joints with respect to the local coordinate system of each body can also be consulted in Chapter 5. However, a brief explanation of the experimental acquisition process is provided in the following paragraph to clarify the application example.

The experimental gait data of one adult female subject (29 years old, 53.3 kg) with no history of gait disorders was acquired at the Lisbon Biomechanics Laboratory, located at *Instituto Superior Técnico*. The laboratory is equipped with an optoelectronic motion capture system and three force plates. Prior to data acquisition, the subject had a period of adaptation to the experimental setup. A 15-second static trial was performed, followed by a dynamic trial, in which the subject was asked to walk continuously with her natural cadence. The obtained experimental data was processed and utilized to calculate the joint angles and the coordinates of a biomechanical model, including the position of the center of mass and the Euler parameters of each body, which are necessary to prescribe the experimental data to the model.

In this section, a three-dimensional biomechanical multibody model implemented in MUBODYNA is considered to demonstrate the application of the driving constraints formulation. The developed model corresponds to the right human lower limb, and it is composed of five rigid bodies, including the pelvis, thigh, leg, main foot and toes. These bodies are kinematically connected to each other by means of four joints, namely one spherical joint connecting the pelvis to the thigh and representing the hip joint, one revolute joint linking the thigh to the leg and mimicking the knee joint, one modified universal joint connecting the main foot to the leg and representing the ankle joint complex, and one revolute joint linking the toes to the main foot and mimicking the metatarsophalangeal joint. Hence, the developed biomechanical model has 13 degrees-of-freedom, which correspond to the flexion/extension of the toes, inversion/eversion of the main foot, plantarflexion/dorsiflexion of the main foot, flexion/extension of the leg, and flexion/extension, adduction/abduction and internal/external rotation of the thigh. The remaining six degrees-of-freedom represent the translation and rotation of the biomechanical multibody model as a whole. The designation of the bodies and joints, and the location of the centers of mass of each body are shown in Figure 3.38.

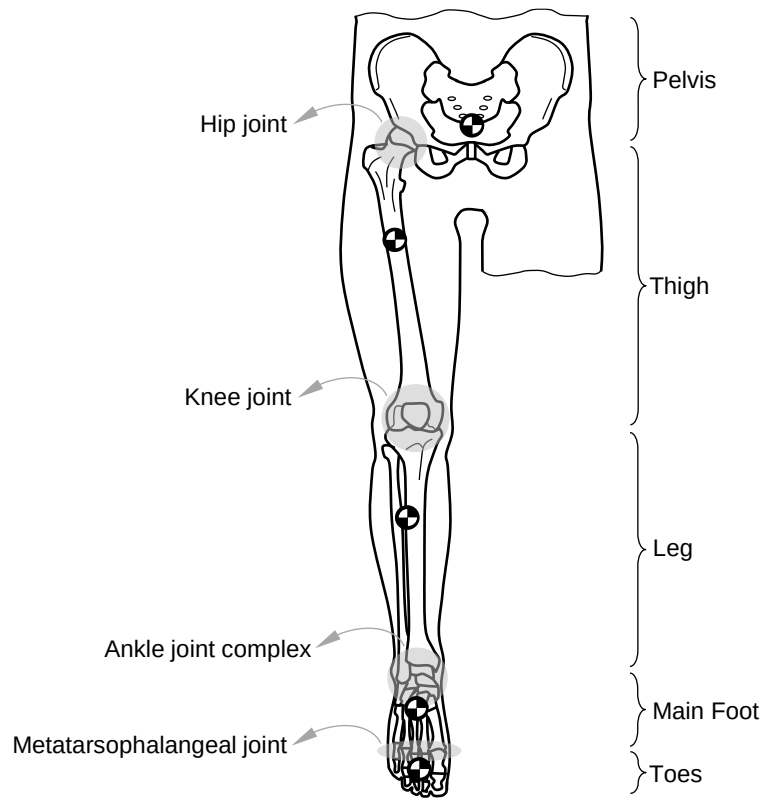
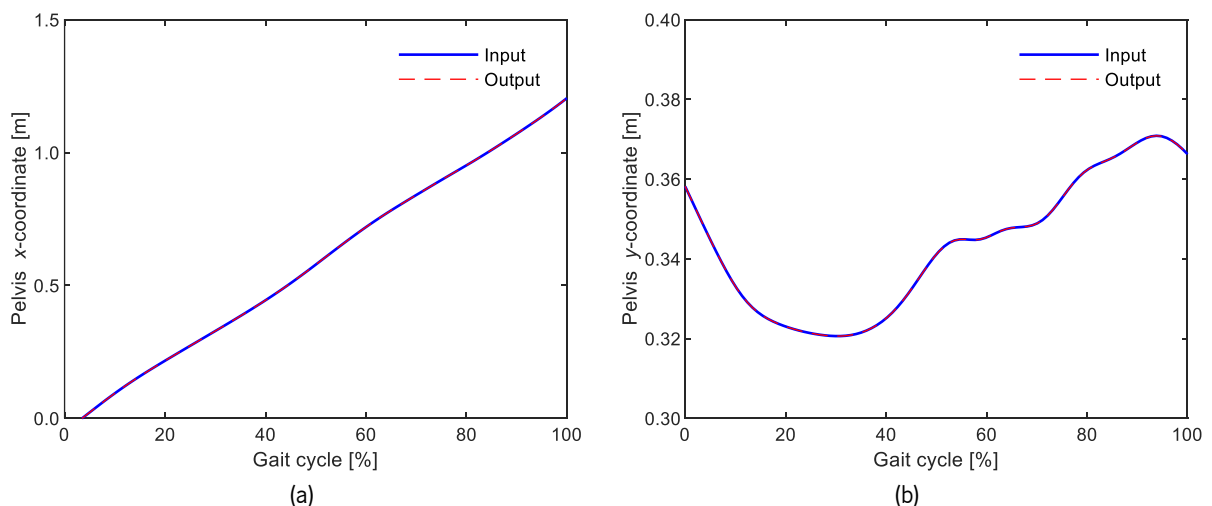


Figure 3.38 – Schematic representation of the biomechanical multibody model of the right human lower limb.

The 13 degrees-of-freedom of the biomechanical multibody model are guided using the experimentally acquired data and the formulation of the driving constraints described in section 3.4. In this example, the trajectory of the center of mass, as well as the Euler parameters of the pelvis are guided using Eqs. (3.67)-(3.74) and (3.75)-(3.81), respectively. The e_1 , e_2 and e_3 Euler parameters are guided. The calculation of the location of the center of mass and the Euler parameters of the pelvis is explained in Chapter 5. Figure 3.39 presents a comparison of the data provided as input to the model using the experimental data and the output data calculated by the model after the process described in Figure 3.2. The input and output data is superimposed, validating the tested driving constraints formulation.



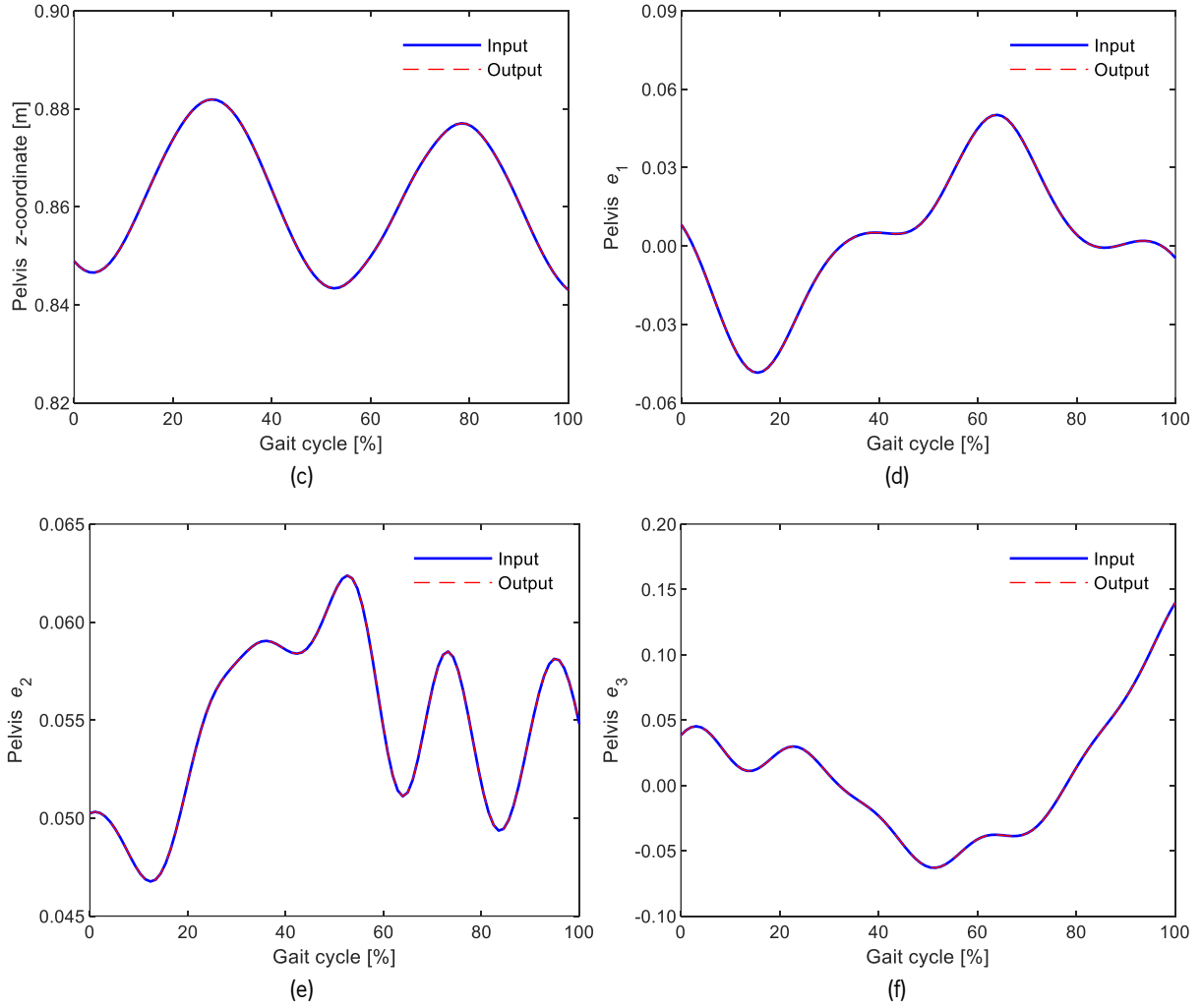


Figure 3.39 – Comparison of the input and output data for the (a) x -coordinate, (b) y -coordinate and (c) z -coordinate for the center of mass, and Euler parameters (d) e_1 , (e) e_2 and (f) e_3 of the pelvis.

The remaining degrees-of-freedom denote the joint angles of the model. The definition of vectors for the application of the driving constraints to guide each angle is explained in the following paragraphs.

As previously described, the knee and the metatarsophalangeal joints are formulated as revolute joints, and, thus Eqs.(3.82)-(3.89) must be applied to guide the joints' angle. The value of $\theta^*(t)$ is calculated using the experimentally acquired data and the inverse cosine function as

$$\theta^*(t) = \arccos(\mathbf{a}_i^T \mathbf{b}_j) \quad (3.132)$$

where vectors $\mathbf{a}_i$ and $\mathbf{b}_j$ are calculated using the experimental data.

It is important to note that the trigonometric function of Eq. (3.132) returns values in the closed interval $[0, \pi]$, and, therefore, vectors $\mathbf{a}_i$ and $\mathbf{b}_j$ must be chosen so that the codomain of the function is not exceeded. If the vectors are defined so that they exceed the codomain, discontinuities in the plot of the joint angle occur, proving incorrect results. An example of this issue is provided in Figure 3.41 for the calculation of the metatarsophalangeal joint angle, in which vectors $\mathbf{a}_i$ and $\mathbf{b}_j$ are expressed as

$$\mathbf{a}_i = \tilde{\mathbf{s}}_{\text{metatarsophalangeal},i} \zeta_i \quad (3.133)$$

$$\mathbf{b}_j = \tilde{\mathbf{s}}_{\text{metatarsophalangeal},j} \zeta_j \quad (3.134)$$

In this situation, vectors $\mathbf{a}_i$ and $\mathbf{b}_j$ are defined with respect to the local coordinate system of the toes (body i) and the main foot (body j), respectively. Vector $\mathbf{s}_{\text{metatarsophalangeal}}$ represents the metatarsophalangeal joint axis vector expressed in the toes or main foot local coordinate system and described in detail in Chapter 5.

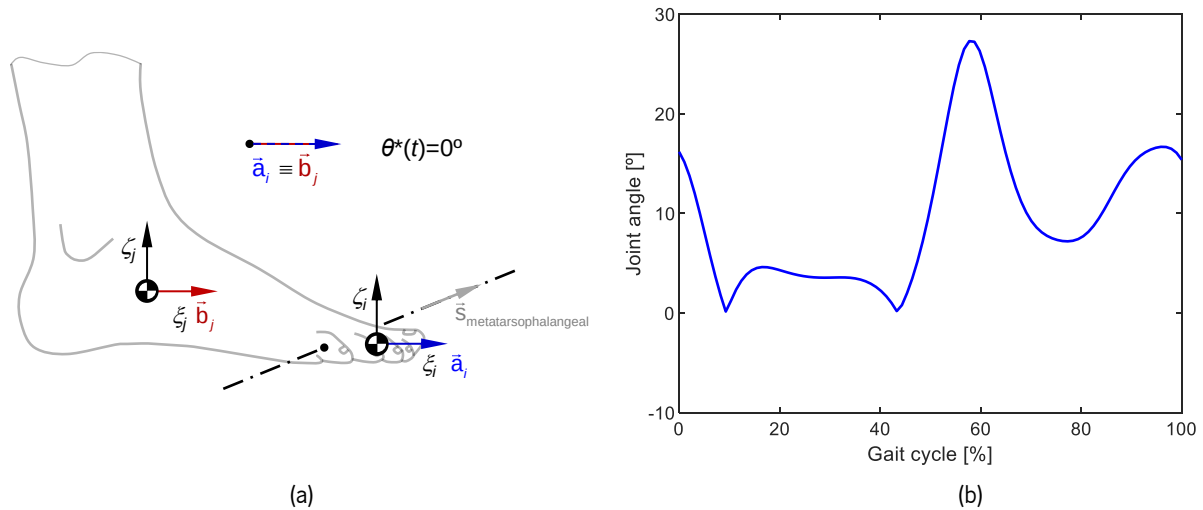


Figure 3.40 – Calculation of the metatarsophalangeal joint angle. (a) Definition of the vectors $\mathbf{a}_i$ and $\mathbf{b}_j$ that exceed the codomain of the inverse cosine function and (b) the corresponding metatarsophalangeal joint angle.

In this work, in order to overcome this issue, the vectors utilized to calculate $\theta^*(t)$ are defined such that vector $\mathbf{a}_i$ is rotated 90 degrees relative to Eq. (3.133). This solution is now applied to the calculation of the metatarsophalangeal joint angle, as it can be observed in Figure 3.41. In this situation, vector $\mathbf{b}_j$ is given by Eq. (3.134), and vector $\mathbf{a}_i$ is defined as

$$\mathbf{a}_i = \tilde{\zeta}_i \mathbf{s}'_{\text{metatarsophalangeal},i} \quad (3.135)$$

Nevertheless, it is important to note that this procedure is only utilized to provide the driving constraint to the biomechanical multibody model and to avoid the codomain-related issue. The calculated joint angle does not represent the actual joint angle. In this work, the actual angle is obtained by calculating the joint angles using the static trial, in which the volunteer stands in the anatomical reference position. The angle calculated using the static trial is then subtracted to the one obtained using Eq. (3.132). However, it is important to note that, if the angle does not exceed the codomain of the function, the procedure of rotating the vectors may not need to be carried out. However, in this work, this procedure is utilized to calculate all joint angles in order to guarantee correct results for the considered biomechanical multibody model.

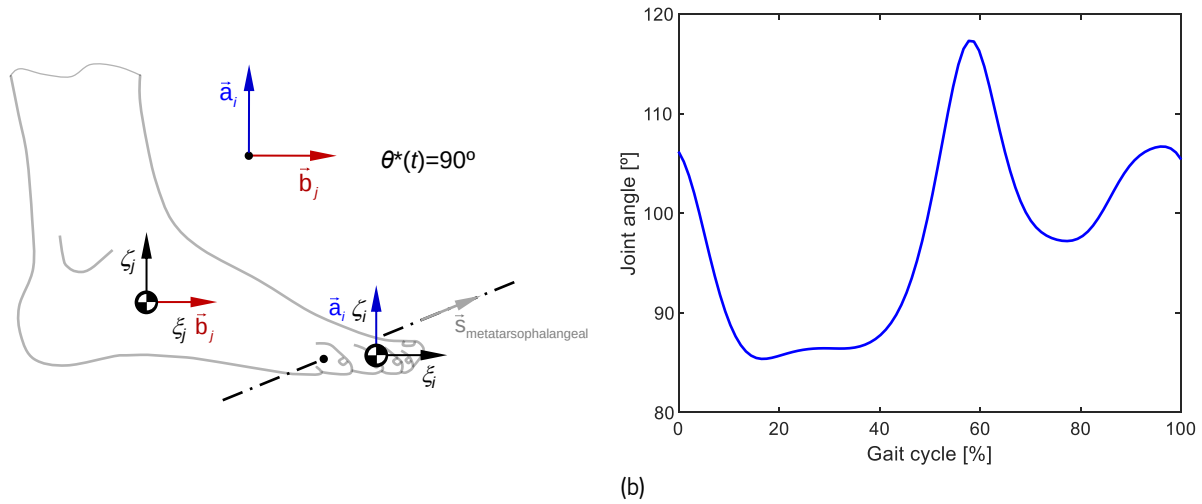


Figure 3.41 – Metatarsophalangeal joint angle. (a) Definition of the vectors $\mathbf{a}_i$ and $\mathbf{b}_j$ that do not exceed the codomain of the inverse cosine function and (b) the corresponding metatarsophalangeal joint angle.

The actual metatarsophalangeal joint angle is obtained by subtracting the angle calculated in the static trial from the curve of Figure 3.41. Hence, Figure 3.42 shows the actual joint angle and compares the value provided as input to the biomechanical model and the value calculated as output after running the process illustrated in Figure 3.2. The fact the two curves of Figure 3.42 are superimposed indicates that the driving constraint of Eqs.(3.82)-(3.89) are properly guiding the metatarsophalangeal joint angle.

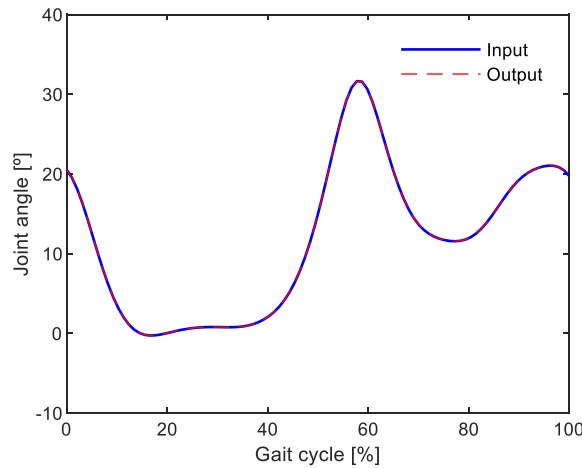


Figure 3.42 – Comparison of the output and input curves of the actual metatarsophalangeal joint angle.

For the calculation of the knee joint angle, the same procedure is carried out and it is illustrated in Figure 3.43. The $\mathbf{a}_i$ and $\mathbf{b}_j$ vectors are expressed, respectively, as

$$\mathbf{a}_i = \tilde{\xi}_i \mathbf{s}_{\text{knee},i} \quad (3.136)$$

$$\mathbf{b}_j = \tilde{s}_{\text{knee},j} \zeta_j \quad (3.137)$$

in which $\mathbf{s}_{\text{knee}}$ denotes the knee joint axis vector expressed in the thigh (body i) and leg (body j) local coordinate systems.

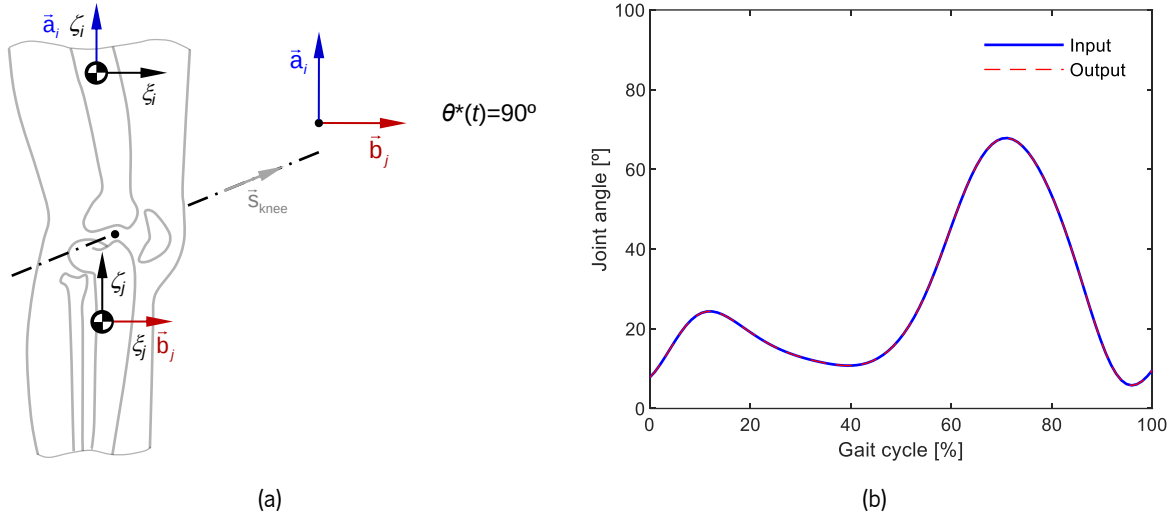


Figure 3.43 – Knee joint angle. (a) Illustration of vectors $\mathbf{a}_i$ and $\mathbf{b}_j$ that do not exceed the codomain of the inverse cosine function and (b) comparison of the output and input curves of the actual knee joint angle.

Concerning the talocrural and talocalcaneal joints, Eqs.(3.91)-(3.102) must be considered since the ankle joint complex is formulated as a modified universal joint. For the talocrural and talocalcaneal joints, vector $\mathbf{d}_p$ represents the projection of massless link vector onto the plane perpendicular to the $\mathbf{s}_{\text{talocrural}}$ and $\mathbf{s}_{\text{talocalcaneal}}$ joint axis, respectively. In addition, similarly to the metatarsophalangeal and knee joints, the inverse cosine trigonometric function is utilized to calculate the joint angle $\varphi^*(t)$ as

$$\varphi^*(t) = \arccos\left(\frac{\mathbf{a}_i^T \mathbf{d}_p}{\|\mathbf{d}_p\|}\right) \quad (3.138)$$

where vectors $\mathbf{a}_i$ and $\mathbf{d}_p$ are calculated using the experimental data.

The previously described procedure of rotating the vector $\mathbf{a}_i$ to avoid the codomain-related issue is also employed in this situation. Therefore, vector $\mathbf{a}_i$ is expressed as

$$\mathbf{a}_i = \tilde{\mathbf{s}}_{\text{talocrural},i} \zeta_i \quad (3.139)$$

for the talocrural joint and as

$$\mathbf{a}_i = \tilde{\zeta}_i \mathbf{s}_{\text{talocalcaneal},i} \quad (3.140)$$

for the talocalcaneal joint. It is important to note that body i denotes the leg and the main foot for the talocrural and talocalcaneal joints, respectively.

Figure 3.44 presents a schematic representation of the vectors utilized to calculate the talocrural and the talocalcaneal joint angles, as well as a comparison containing the plots of the actual joint angles provided as input to the biomechanical multibody model and as the calculated output. The actual joint angles are calculated following the same procedure used for the metatarsophalangeal and knee joints.

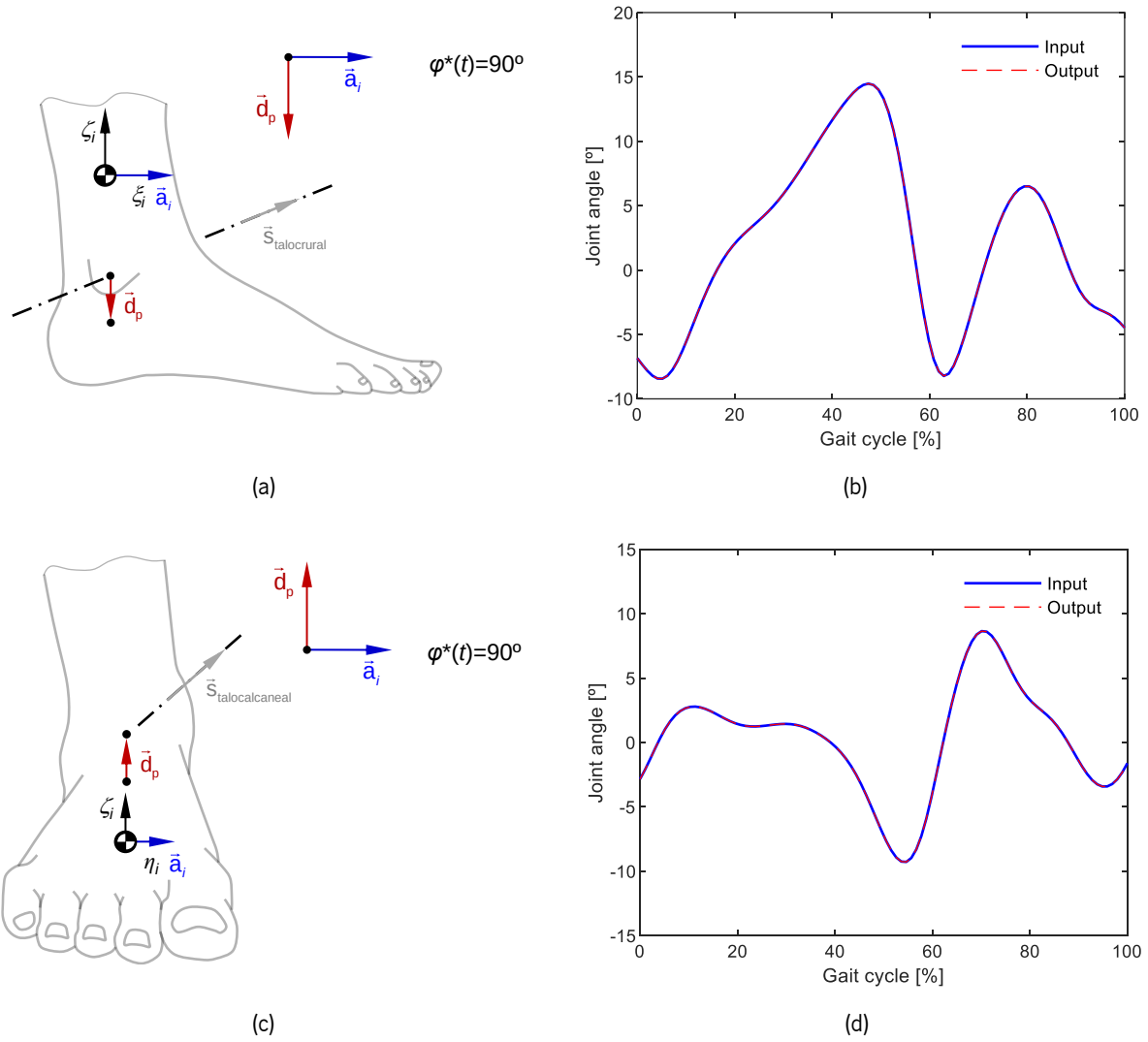


Figure 3.44 – Talocrural and talocalcaneal joint angles. Illustration of vectors $\mathbf{a}_i$ and $\mathbf{d}_p$ utilized to calculate the (a) talocrural and (c) talocalcaneal joint angles, and comparison of the output and input curves of the actual (b) talocrural and (d) talocalcaneal joint angles.

Finally, for the hip joint formulated as a spherical joint in the biomechanical multibody model, Eqs. (3.103)–(3.121) must be utilized to guide joint angles in the sagittal, frontal, and transverse planes. The joint angle in each plane is calculated as

$$\phi^*(t) = \arccos\left(\frac{\mathbf{a}_i^T \mathbf{b}_{j,p}}{\|\mathbf{b}_{j,p}\|}\right) \quad (3.141)$$

in which vectors $\mathbf{a}_i$ and $\mathbf{b}_{j,p}$ are defined using the experimental data.

For the sagittal and frontal planes, the vector connecting the center of mass of the thigh (body j) to the knee joint, $\mathbf{s}_{\text{CoM,knee}}$, is utilized as vector $\mathbf{b}_j$, and it is expressed as

$$\mathbf{b}_j = \mathbf{s}_{\text{CoM,knee}} \quad (3.142)$$

The definition of this vector is extracted from anthropometric databases, and it is described in detail in Chapter 5. Vector $\mathbf{b}_j$ is then projected on the sagittal and frontal planes, using the condition of Eq. (3.104), where vector $\mathbf{s}_i$ is expressed as

$$\mathbf{s}_i = \boldsymbol{\eta}_i \quad (3.143)$$

for the sagittal plane and as

$$\mathbf{s}_i = \boldsymbol{\xi}_i \quad (3.144)$$

for the frontal plane. The pelvis is considered to be body i (see Figure 3.45a and c).

Vector $\mathbf{a}_i$ is expressed for the sagittal and frontal planes, respectively, as

$$\mathbf{a}_i = \boldsymbol{\xi}_i \quad (3.145)$$

$$\mathbf{a}_i = \boldsymbol{\eta}_i \quad (3.146)$$

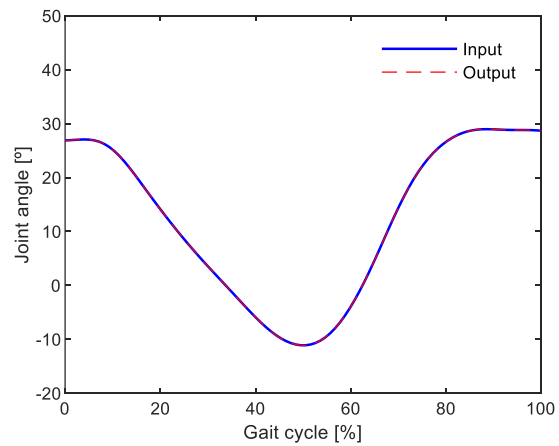
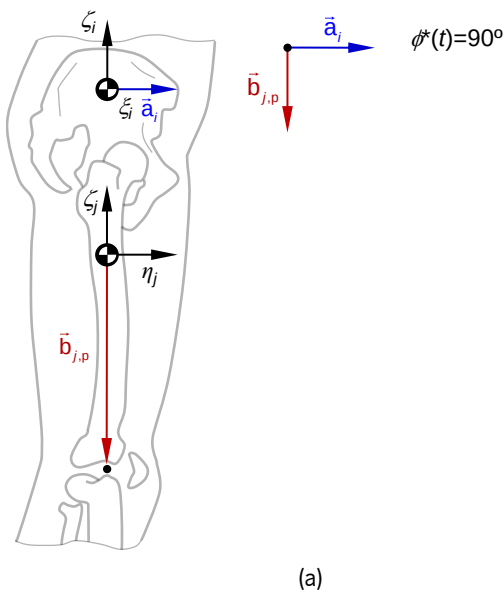
For the transverse plane, Eq. (3.146) is utilized for vector $\mathbf{a}_i$. In turn, vector $\mathbf{b}_j$ of Eq. (3.142) must be rotated 90 degrees in order to be utilized to calculate the internal/external rotation of the hip joint as (see Figure 3.45)

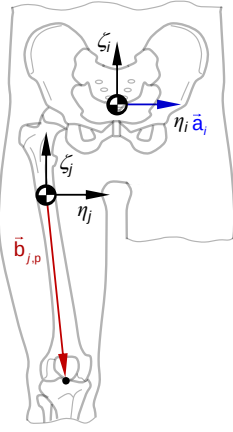
$$\mathbf{b}_j = \tilde{\mathbf{s}}_{\text{CoM,knee}} \boldsymbol{\eta}_i \quad (3.147)$$

Vector $\mathbf{b}_j$ is then projected on the transverse plane using Eq. (3.104), where vector $\mathbf{s}_i$ is as

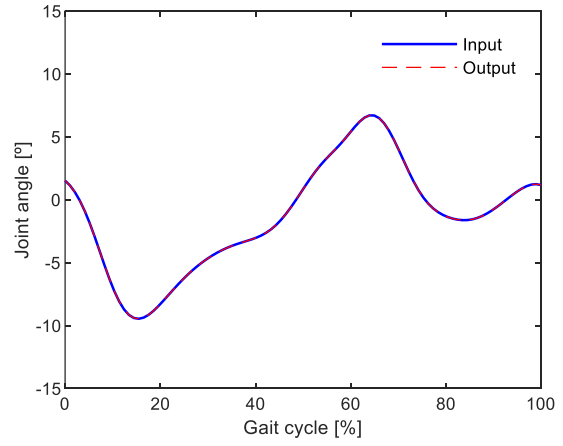
$$\mathbf{s}_i = \boldsymbol{\zeta}_i \quad (3.148)$$

Figure 3.45 depicts the vectors $\mathbf{a}_i$ and $\mathbf{b}_{j,p}$ utilized to calculate the hip joint angles. The actual joint angles are calculated using the angles determined in the static trial, following the same procedure utilized for the metatarsophalangeal, knee, talocrural and talocalcaneal joints.

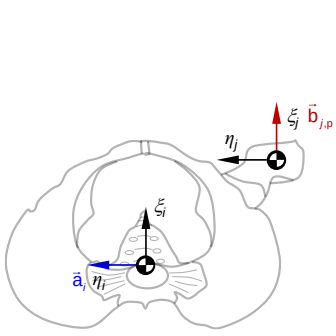




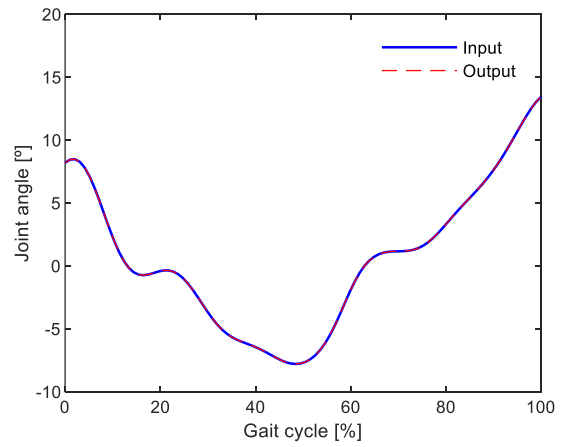
(c)



(d)



(e)



(f)

Figure 3.45 – Illustration of vectors $\vec{a}_i$ and $\vec{b}_{j,p}$ utilized to calculate the hip joint angles in the (a) sagittal, (c) frontal and (e) transverse planes, and representation of the actual hip joint angles in the (b) sagittal, (d) frontal and (f) transverse planes.

As mentioned previously, the main objective of this application example is to validate the proposed formulation for the driving constraints developed in section 3.4. The observation of Figure 3.42 though Figure 3.45, leads to the conclusion that the formulated driving constraints allow to correctly guide the 13 degrees-of-freedom of the biomechanical multibody model analyzed in this example. This conclusion can be drawn from the fact that the input and output curves of the analyzed joint angles are superimposed in all analysis carried out.

The violation of the constraint equations at the position and velocity levels is presented in Figure 3.46. It can be concluded that the magnitude of the constraints violation is negligible, which indicates that all constraints of the biomechanical multibody model, including joint and driving constraints, are not violated throughout the entire analysis. This conclusion allows to further validate the proposed driving constraint formulation.

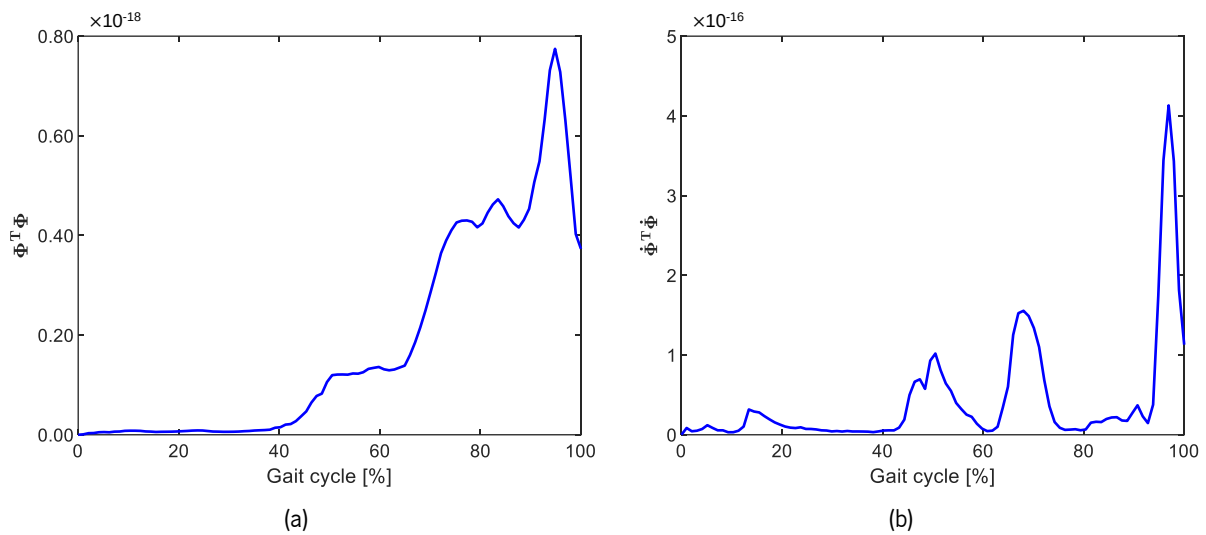


Figure 3.46 – Time variation of the constraints violation at (a) position and (b) velocity levels for the biomechanical multibody model of the human right lower limb.

3.6. Summary and Discussion

In this chapter, the formulations proposed and developed in this work within the framework of multibody systems methodologies are presented and discussed. The chapter begins with a brief explanation of the basic concepts associated with the methodology, which represents the foundation for all the work developed in this chapter. Then, the complete characterization of the novel kinematic joint model to formulate for the ankle joint complex of the human foot, that is, the modified universal joint, is provided. The main kinematic modeling aspects of these two joint approaches were described, taking into account the corresponding kinematic constraints, the resulting Jacobian matrix, and the right-hand side of the acceleration constraint equations vector. A methodology to restrict the range of motion of joints is proposed and thoroughly described. The methodology extends and improves previous works, specifically in what regards to the definition of the range of motion limits, the calculation of the penalty moments and the establishment of their direction of application. Enhanced methods to deal with the detection of unacceptable joint configurations are also proposed. A parametrization procedure of the circumduction cone is described to correctly calculate the direction of the penalty moments to apply to the connected bodies. Afterwards, the driving constraints formulation developed in this work to guide the degrees-of-freedom of the multibody models is established. Five types of driving constraints are proposed and described in detail, which allow to, using experimental data, guide the translation and orientation of a body, as well as to control the angle of the joints of a multibody model. Finally, the performance of the aforementioned formulations is verified at the end of the chapter through the analysis of three application examples. Several modeling issues are addressed, discussed and the proposed formulations validated.

“The brain is like a muscle. When it is in use we feel very good. Understanding is joyous.”

Carl Sagan

4. SKELETAL MUSCLE MODELING

Skeletal muscles produce movement of the human body by receiving signals from the central nervous system and contracting. Besides allowing physiological movements, these muscles also prevent abnormal joint motion and provide joint stability. Skeletal muscles are attached to the bones of the skeletal system by means of tendons located at their ends. The muscular contraction produced by the muscle fibers is transmitted to the tendon during movement, thus producing joint motion. In this chapter, the most important concepts associated with muscle modeling are presented. The anatomy and physiology of skeletal muscles are approached, followed by the explanation of the mechanism by which muscular contraction occurs, including the detailed presentation of the considered mathematical model. The formulation for introducing muscle forces into the equations of motion and the optimization procedure are described. The chapter ends with two application examples incorporating the discussed concepts.

4.1. Skeletal Muscle Anatomy and Physiology

There are three types of muscles in the human body, namely skeletal, cardiac, and smooth muscles (Roupa et al., 2022). However, to the scope of this work, only the anatomy and physiology of skeletal muscles is approached since these are the soft tissues responsible for producing movement of the human body. From a mechanical perspective, the main function of skeletal muscles is to convert chemical energy into mechanical energy in order to generate force and power, maintain posture, and produce joint movement. Skeletal muscles also prevent excessive or abnormal joint motion, promoting skeletal stability and avoiding damage of the surrounding anatomical structures (Frontera & Ochala, 2015; Zatsiorsky & Prilutsky, 2012).

The connection of skeletal muscles to bones is achieved by means of tendons located at their ends. The contraction of skeletal muscles extends to both proximal and distal tendinous attachments, ultimately producing joint motion. The proximal and distal attachments of a muscle to a tendon are known as its origin and insertion, respectively (Yoshimoto & Oishi, 2023). The functional unit that produces joint

motion is termed the muscle-tendon unit (MTU) and it consists of a muscle that has an origin and an insertion, and a tendon or an aponeurosis that interdigitates with the muscle by a musculotendinous junction (Vila Pouca et al., 2021). Figure 4.1 provides a schematic representation of a MTU with its respective muscle and tendon connecting to the bones of the human upper limb.

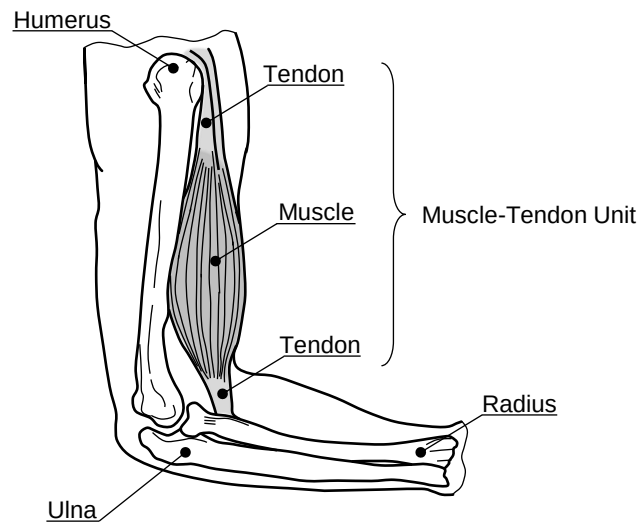


Figure 4.1 – Schematic representation of a muscle-tendon unit connecting to the bones of the human upper limb.

Skeletal muscles present a very complex, yet organized structure. As observed in Figure 4.2, these types of muscles are arranged into a series of structural units of decreasing size, which are enclosed inside one another in a well-defined hierarchical structure. An outer layer of dense connective tissue, called epimysium, covers the muscle and separates it from other neighboring muscles. Underneath the epimysium, skeletal muscles are composed of a set of muscle fascicles. Each fascicle is covered and connected to another by means of a fibrous tissue, designated by perimysium. Muscle fascicles are divided into smaller structures called the muscle fibers, which are long cells composed of smaller units, known as the myofibrils. It is at the muscle fiber level that muscular contraction occurs. The set of muscle fibers are embedded in a thin tubular membrane, called sarcolemma, which is responsible for maintaining an electrical membrane potential essential for muscular contraction. Muscle fibers are surrounded and held together by a layer of collagenous tissue, known as endomysium. The myofibrils are composed of subunits called sarcomeres, arranged end to end in a parallel manner along the entire length of the muscle fiber. Sarcomeres are the functional unit of the muscular contraction, since shortening of each sarcomere generates shortening of the entire muscle fiber. Each sarcomere contains two myofilaments, namely the thin filaments comprising actin proteins and the thick filaments including myosin proteins. Skeletal muscles can also be termed as striated muscles due to the fact that sarcomeres have a typical striated pattern, as observed in Figure 4.2 (Frontera & Ochala, 2015; Neumann, 2013; Oatis, 2008).

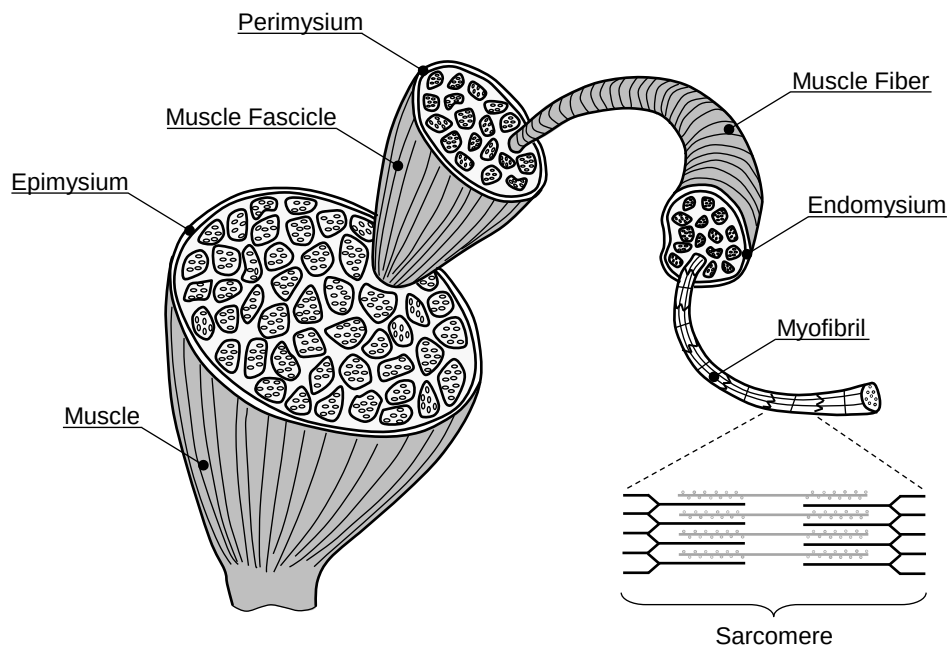


Figure 4.2 – Schematic representation of the hierarchical organization of the skeletal muscle.

Several regions can be identified in the sarcomere, as observed in Figure 4.3. The thin actin filaments are more abundant than the thick myosin filaments, being anchored at both ends of the sarcomere at the Z-line and projected to interior of the sarcomere, where they surround the myosin filaments. The Z-line is a protein sheet and the distance between two adjacent Z-lines corresponds to the sarcomere length. The darker region of the sarcomere or A-band extends to the length of the myosin filaments. The region of the sarcomere containing actin filaments only is called I-band or light region. In the H zone there is no superimposition of the two myofilaments, containing myosin filaments only. In the middle of this zone there is the M-line, containing the proteins strands that hold together the myosin filaments. Titin is a protein connecting the myosin to the Z-line (Oatis, 2008; Zatsiorsky & Prilutsky, 2012).

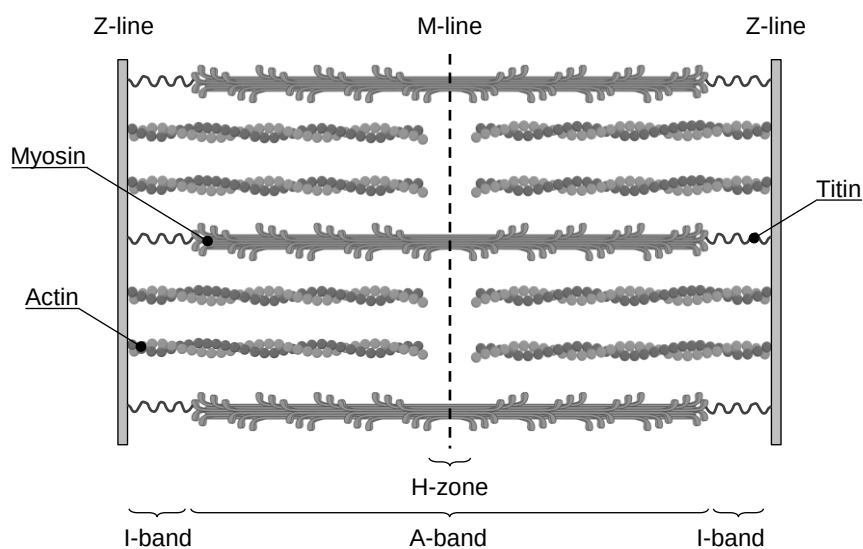


Figure 4.3 – Schematic representation of the structure of a sarcomere.

Muscle fibers exert forces along their longitudinal axes, while MTUs exert forces along tendons. The arrangement of fibers in skeletal muscles varies significantly and influences their ability to produce movement and generate force (Hall, 2012; Zatsiorsky & Prilutsky, 2012). According to their morphology, muscles can be broadly classified as fusiform or pennate. In fusiform muscles, such as the biceps brachii, the fibers are oriented largely in parallel with the longitudinal axis of the muscle and tendon. In turn, in pennate muscles, such as the rectus femoris, the fibers insert obliquely into the tendon. The angle at which muscle fibers insert at a tendon is called the pennation angle, α , as illustrated in see Figure 4.4. Depending on the number of similarly angled set of muscles fibers attaching into the tendon, pennate muscles can be further classified as unipennate, bipennate or multipennate. Due to this arrangement, the direction of an individual muscle fiber force and the direction of the tendon force are different (Hall, 2012; Neumann, 2013; Oatis, 2008; Zatsiorsky & Prilutsky, 2012).

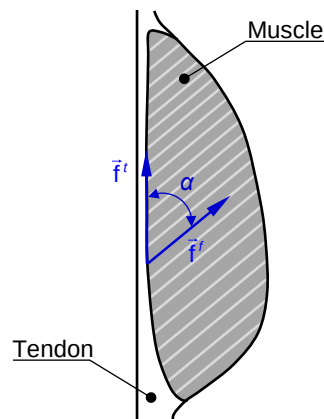


Figure 4.4 – Schematic representation of the pennation angle established between the muscle fibers and the tendon.

When a parallel-fibred muscle contracts, the shortening of the muscle is primarily the result of the shortening of its fibers, allowing greater shortening of the entire muscle. On the contrary, in pennate muscles, the shortening of the fibers provokes the rotation about their tendon attachment, progressively increasing the pennation angle. The greater the pennation angle, the smaller the amount of effective force transmitted to the tendon to produce joint motion as

$$f^t = f^f \cos \alpha \quad (4.1)$$

where f^t and f^f are the tendon and fiber forces, respectively, and α represents the pennation angle.

Although pennation reduces the effective muscle force, this arrangement allows the packing of more fibers into a given muscle volume. Hence, the total force produced by the muscle fibers can be greater than that of parallel-fibred muscles of the same volume. However, only a component of fiber force contributes to the muscle force in pennate muscles due to the oblique orientation of the fibers with respect to the tendon (Hall, 2012; Zatsiorsky & Prilutsky, 2012).

The contraction of skeletal muscles is voluntary, which means that it occurs under the control of the central nervous system through electrochemical stimuli. The excitation-contraction coupling is the term utilized to describe the sequence of occurrences that begin with the generation of the neural signal from the central nervous system and ends with the muscular contraction (Calderón et al., 2014; Shishmarev, 2020). The neural signal is propagated through specialized cells, named motoneurons, until reaching the muscle fibers. The set formed by a motoneuron and the individual muscle fibers it innervates is termed motor unit. The neural signal sent by the nervous system stimulates the muscle fibers, activating them, which are then capable of contracting and producing a muscle force (Rodríguez Cruz et al., 2020).

Motoneurons possess at their terminations structures called axon terminals, which connect the motoneuron to the muscle fiber. To the connection between an axon terminal and a muscle fiber is given the name of neuromuscular junction (Rodríguez Cruz et al., 2020). A muscle is stimulated when a neural signal from a motoneuron arrives at the neuromuscular junction. This muscular stimulation causes the neurotransmitter acetylcholine (ACh), which is contained within vesicles, to be released into the synaptic cleft, which is a small gap between the axon terminals and the muscle fiber. The ACh is responsible for muscle fiber activation, disseminating across the synaptic cleft and binding to specialized receptors on the muscle fiber membrane, the sarcolemma. This phenomenon provokes a local depolarization of the fiber membrane, which rapidly propagates to the entire muscle, provoking the release of calcium ions that will take part in the muscular contraction process occurring at sarcomere level. The calcium ions (Ca^{2+}) bind to a protein called troponin, causing the thin actin filaments to bind to the thick myosin filaments forming crossbridges, beginning the contraction of the muscle. According to the sliding filament theory, contraction occurs by the sliding of the thin actin filaments over the thick myosin filaments, shortening the I-band and H-zone, while the length of the A-band remains constant (see Figure 4.3). The force produced by the muscle is transmitted to its adjacent tendon, which, in turn, transmits the force to the bone, resulting in joint motion. When the neural signal ends, the concentration of calcium ions within the muscle fibers reduces, inhibiting the crossbridges between the two myofilaments and causing the muscle to relax (Frontera & Ochala, 2015; Oatis, 2008; Zatsiorsky & Prilutsky, 2012).

Figure 4.5 shows the processes occurring from neural signal generation until the production of muscular force. In this work, only the muscular contraction is approached in the following sections.

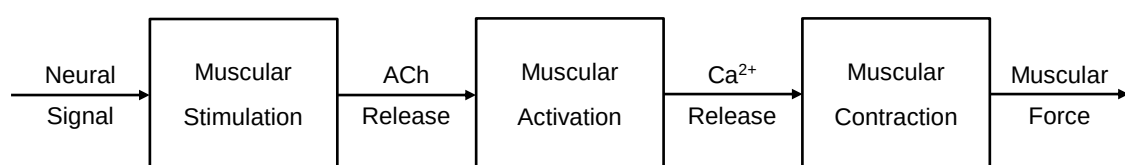


Figure 4.5 – Sequence of events occurring from neural signal generation until the production of muscular force.

The muscular force production is influenced (i) by the frequency of neural signals that arrive at the muscle fibers and (ii) by the recruitment of additional motor units, of larger size (M. T. Silva, 2003). Regarding the first process, if a single neural signal of low intensity reaches the motoneuron, a twitch contraction occurs (see Figure 4.6a). If the frequency of the signal increases, the twitch contraction repeats. If this repetition occurs before the muscle has time to relax, it tends to add up. To this process is given the name of summation (see Figure 4.6b). The increase in the stimulation frequency tends to reduce the time gap occurring between two consecutive twitches. Since the muscle has no time to fully relax before the subsequent twitch arises, they add up. If the frequency of stimuli continues to increase, the muscle contraction reaches its peak force and plateaus at that level, producing a tetanic contraction (see Figure 4.6c). As the tetanic contraction is prolonged, fatigue occurs, which causes a gradual decline in the level of muscle force produced (see Figure 4.6d). It is important to consider that, in all cases, there is a time delay between the occurrence of the neural stimulus and the initiation of muscular contraction, which is called latent period and corresponds to the time that the neural stimulus takes to be propagated along the muscle fibers (Hall, 2012; M. T. Silva, 2003).

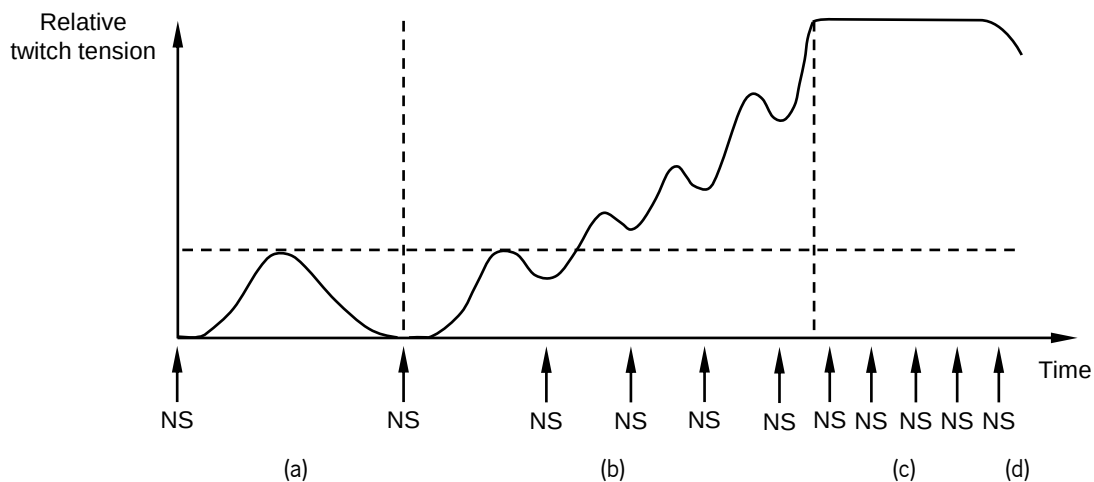


Figure 4.6 – Events occurring when a muscle is stimulated. a) Twitch. b) Summation. c) Tetanus. NS – neural signal.

After being stimulated, some muscle fibers may contract quicker than others. Based on this response to neural signals, muscle fibers are classified as fast twitch and slow twitch. It takes fast twitch fibers about one-seventh the time required by the slow twitch fibers to reach the maximum force magnitude. A motor unit comprises the same type of fibers, either fast or slow twitch. However, most skeletal muscles possess both slow and fast twitch fibers, with the relative amounts varying considering the muscle and the subject. In events requiring fast, powerful muscular contractions, for instance, sprinting or jumping, fast twitch fibers are very important. In turn, in actions related to endurance testing, such as distance running, slow twitch muscles are required (Hall, 2012).

Muscles have different functions during movement. When a muscle contracts and provokes movement of a body segment at a joint, it is acting as an agonist. In contrast, muscles with action opposite to those of the agonists are called antagonists and exert eccentric force at the same time the agonists are causing movement. Agonists and antagonists are typically positioned in opposite sides of joints.

4.2. Muscle Contraction Dynamics

As explained in the previous section, to the scope of this work, only the muscle contraction dynamics, which corresponds to the transformation of the muscle activation into muscle force production, is approached (Buchanan et al., 2004). According to macroscopic muscle length alterations, there are three types of muscular contractions, namely isometric, concentric, and eccentric contractions. An isometric contraction does not alter the length of the muscle, while in concentric and eccentric contractions the macroscopic muscle length diminishes and increases, respectively (Neumann, 2013).

Mathematical models are utilized to relate the force produced by a skeletal muscle with the resulting movement of the musculoskeletal system (Yamaguchi, 2001). There are two main types of mathematical models to simulate the muscle contraction dynamics, namely the physiological models and the phenomenological models. Physiological models tend to be very complex, and the muscle dynamics is governed by multiple differential equations that must be numerically integrated, penalizing the computational efficiency (Buchanan et al., 2004). Examples of physiological models include the Huxley (1958) and the Huxley & Simmons (1971) models. In turn, phenomenological models characterize the external behavior of the muscle, instead of the underlying physiology. Phenomenological models can further be classified as passive or active models. Passive models, including the Maxwell, the Voight, or the Kelvin models (see Figure 4.7), utilize spring and damper elements to simulate the behavior of muscles under compressive and tensile loads. However, passive models are not capable of representing the dynamics of the muscle contractile structures, which is an essential part of muscle modeling. In order to overcome this issue, Hill (1938) introduced an adaptation to the Kelvin muscle model, in which the active muscle behavior is properly described using a contractile element (see Figure 4.7). The contractile element allows to simulate, at a macroscopic level, the active muscle action produced by the sarcomeres, in particular, the crossbridge formation during muscular contraction. Since it is an evolution of the Kelvin model, the Hill model is also capable of accurately simulating the passive behavior of the muscle. For this purpose, it has a parallel damping element simulating the viscous force produced by the intracellular and intercellular fluid within the muscle, a parallel elastic element that accounts for the non-linear passive properties of the tissues surrounding the muscle, i.e. the perimysium, and a series elastic element

simulating the elasticity of the actin-myosin crossbridges (M. T. Silva, 2003; Yamaguchi, 2001). One advantage of Hill-type muscle models is that the muscle dynamics is governed by one differential equation per muscle, increasing the computational efficiency when compared with physiological models (Buchanan et al., 2004). Passive and active elements can be combined depending on the simulated behavior. A representation of the passive and active phenomenological muscle models is provided in Figure 4.7.

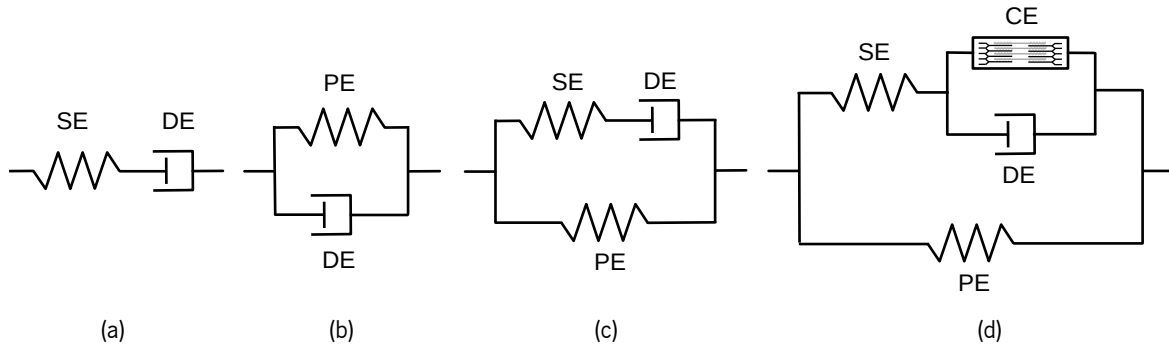


Figure 4.7 – Schematic representation of phenomenological muscle models. (a) Maxwell, (b) Voigt, (c) Kelvin and (d) Hill. The abbreviations CE, DE, PE, and SE refer to contractile, damping, parallel elastic, and series elastic elements, respectively.

The muscle model utilized in this work is a variant of the Hill model (Hill, 1938) and it is illustrated in Figure 4.8a. The model is composed of an active contractile element, which includes the properties of both the contractile and the damping elements, arranged in parallel with an elastic element. According to Zajac (1989), the energy stored in crossbridges is expected to be very small in comparison with the energy stored in tendons. Thus, with the exception of short-tendon actuators, tendon compliance is predominant over muscular crossbridge compliance, and the series elastic element can be neglected. Consequently, in this work, the contribution of the series elastic element is not considered. Henceforth, for simplicity reasons, the term muscle is utilized to refer to the muscle fibers.

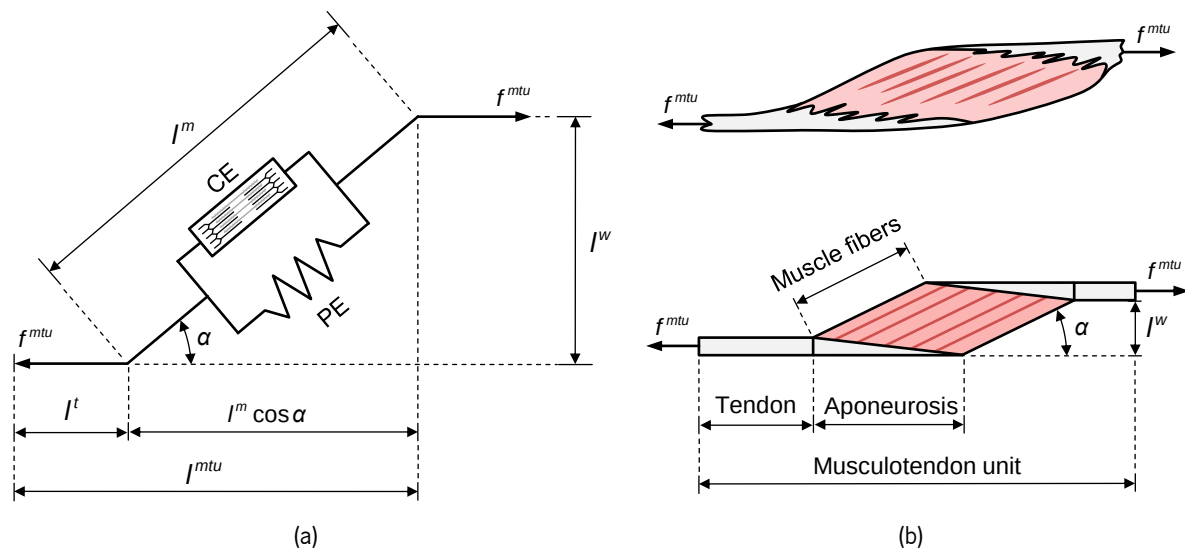


Figure 4.8 – Schematic representation of the (a) computational and (b) physiological Hill-type muscle model utilized to simulate the contraction dynamics. The abbreviations CE and PE refer to the contractile and parallel elastic elements, respectively.

In the model presented in Figure 4.8, the muscle actuator is influenced by the pennation angle, α , in order to accommodate oblique muscle insertions. As observed in Figure 4.8b, the pennation angle represents the angular orientation that the muscle fibers present with respect to the aponeurosis, that is, the internal portion of the tendon. The model assumes that all muscle fibers that constitute a given muscle are straight and coplanar, have the same length l^m and have parallel orientation relative to each other. Additionally, it is also considered that the MTU is massless and frictionless (Oliveira et al., 2016). The MTU length, l^{mtu} , varies according with the kinematics of the movement under analysis and results from the sum of the tendon length, l^t , and the length of the muscle, l^m , taking into consideration the pennation angle, and can be expressed by the following condition

$$l^{mtu} = l^t + l^m \cos \alpha \quad (4.2)$$

Due to the fact that the muscle and the tendon are assembled in series, as observed in Figure 4.8, the resultant MTU force is equal to the tendon force, which, in turn, is equal to the force produced by the muscle projected onto the line of action of the tendon. Moreover, in this work, the tendon is assumed to be rigid, and, thus, to the force produced by MTU contributes exclusively the force produced by the muscle as

$$f^{mtu} = f^t = f^m \cos \alpha \quad (4.3)$$

where f^{mtu} , f^t and f^m are the force of the MTU, tendon and muscle, respectively, and α is calculated as

$$\alpha = \arctan\left(\frac{l^w}{l^{mtu} - l^t}\right) \quad (4.4)$$

in which l^w is the muscle width estimated as

$$l^w = l_0^m \sin \alpha_0 = l^m \sin \alpha \quad (4.5)$$

where l_0^m corresponds to the muscle optimal length.

For the calculation of the muscle width, the constant isovolume assumption is considered, which assumes that the muscle maintains the same volume as the muscle fibers shorten. For Eq. (4.5) to be valid, the MTU model must consider that the aponeurosis thickness increases from the internal to the external portion of the tendon, as depicted in Figure 4.8b, such that all muscle fibers are parallel and equal in length (Zajac, 1989).

Both the contractile and the parallel elastic elements contribute to the total muscle force, f^m , as

$$f^m = f_{PE}^m + f_{CE}^m \quad (4.6)$$

where f_{PE}^m and f_{CE}^m represent the force of the parallel elastic and contractile elements, respectively.

The force of the passive element is exclusively dependent on the muscle length, l^m , and it is only produced when the muscle is stretched beyond its optimal length, l_0^m . The condition utilized to calculate the force of the passive element is obtained from isometric contractions performed with different muscle lengths and it is expressed as (see Figure 4.9) (Kaplan, 2000; M. T. Silva, 2003)

$$f_{PE}^m = \begin{cases} 0 & l^m < l_0^m \\ 8 \frac{f_0^m}{(l_0^m)^3} (l^m - l_0^m)^3 & l_0^m \leq l^m \leq 1.63l_0^m \\ 2 f_0^m & l^m > 1.63l_0^m \end{cases} \quad (4.7)$$

in which f_0^m denotes the maximum isometric muscle force, which corresponds to the force the muscle is capable of producing at its optimal length, l_0^m .

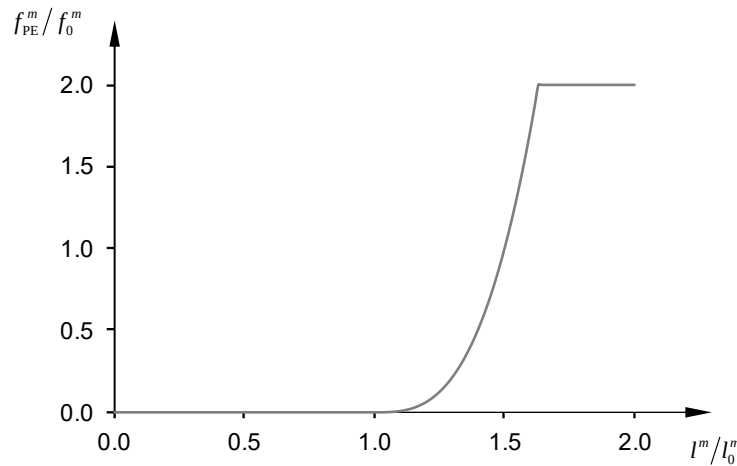


Figure 4.9 – Schematic representation of the force produced by the passive element.

Observing Figure 4.9, it can be concluded that, for muscle lengths shorter than the optimal length, the passive element does not produce force. In this situation, the muscle is in a slack state. However, for muscle lengths longer than the optimal length, the force progressively increases until reaching a maximum magnitude (Neumann, 2013; Oatis, 2008).

In turn, the force produced by the contractile element is dependent on the muscle activation, a^m , on the maximum isometric muscle force, f_0^m , and on the muscle length, l^m , and velocity, v^m , as

$$f_{CE}^m = \frac{f_l^m f_v^m}{f_0^m} a^m \quad (4.8)$$

where f_l^m and f_v^m are two functions representing the muscle force-length and force-velocity relations, respectively. These two relations establish that the maximum contraction force that a skeletal muscle can produce depends on its current length and shortening velocity (M. T. Silva, 2003).

If the muscle activation is disregarded from Eq. (4.8), the remaining terms represent the available force produced by the contractile element, which can be expressed by the following condition

$$\hat{f}_{CE}^m = \frac{f_l^m f_v^m}{f_0^m} \quad (4.9)$$

where the symbol ' $\wedge$ ' represents the available force.

As explained in the previous section, muscular contractions occur at sarcomere level and result from the establishment of crossbridges between the thick myosin and the thin actin filaments, that is, actin from either side of the sarcomere slides over myosin. Due to this sliding of thin filaments over thick filaments, their individual total length remains constant during muscular contraction (Hall, 2012; Oatis, 2008; M. T. Silva, 2003). The force-length relation of the contractile element is a result of the degree of overlap between the actin and myosin filaments. Thus, the number of crossbridges established during muscular contraction is proportional to the force produced by the contractile element. The muscle optimal length represents the length that allows the greatest number of crossbridges and, therefore, the maximum force. As the sarcomere is lengthened or shortened from the optimal length, the number of potential crossbridges decreases and less active force is generated (Oatis, 2008). During isometric contraction, a muscle can only generate force for lengths between approximately half and one and a half times its optimal length. At the optimal length, the maximum force is produced. The resulting force-length curve is described by an inverted U-shape peaking at the muscle optimal length, as observed in Figure 4.10, and it is described by the following condition (Kaplan, 2000; M. T. Silva, 2003)

$$f_l^m = f_0^m e^{\left(-\left[\frac{9\left(\frac{l_m}{l_0^m} - \frac{19}{20} \right)}{4} \right]^4 - \frac{1}{4} \left[\frac{9\left(\frac{l_m}{l_0^m} - \frac{19}{20} \right)}{4} \right]^2 \right)} \quad (4.10)$$

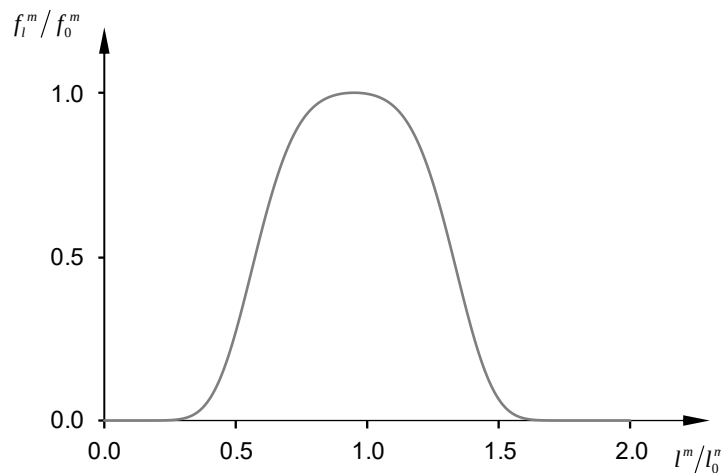


Figure 4.10 – Schematic representation of the force-length relation for the contractile element considering a fully activated skeletal muscle, i.e., $\alpha=1$.

The combination of the passive (see Figure 4.9) and the contractile (see Figure 4.10) force-length relations, yields the total force-length relation of the skeletal muscle (see Figure 4.11), which allows for a wider range of muscle forces over a larger range of muscle length. At lengths below the muscle optimal length, the contractile force dominates. As the muscle is lengthened, the force produced by the contractile element continues to increase until a peak is reached at the muscle optimal length. As the muscle is lengthened beyond its optimal length, the force produced by the passive element begins to contribute. Thus, the decrease in the force produced by the contractile element is compensated by the increase in the force produced by the passive element, which allows the muscle to maintain high levels of force even when the muscle is stretched to a point at which contractile force generation is compromised. As the muscle is further lengthened, the force produced by the passive element dominates (Neumann, 2013).

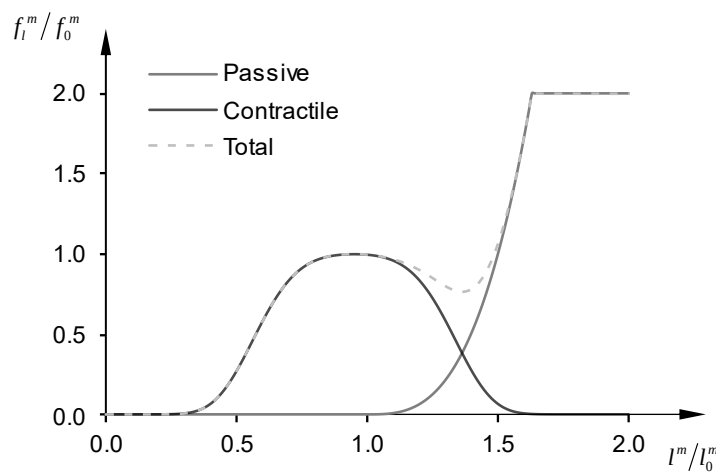


Figure 4.11 – Graphical representation of the force-length relation of a skeletal muscle comprising the passive, contractile and total components. The muscle is considered to be fully activated, i.e., $a^m = 1$.

The capacity of the contractile element to generate force is also dependent on the muscle contraction velocity. The force-velocity relation of the contractile element is represented in Figure 4.12. Positive values for muscle velocity correspond to muscle lengthening, that is, eccentric contractions, while negative values for muscle velocity represent muscle shortening, that is, concentric contractions. The muscle cannot produce force for velocities lower than the maximum contractile velocity, v_0^m . During concentric contractions, that is, the muscle produces force while shortening, the force generated by the contractile element with the same level of muscular activation is smaller than that of an isometric contraction, which is the force produced when v^m is null. During concentric contractions, the produced muscle force is inversely proportional to the contraction velocity. In turn, in the case of an eccentric contraction, that is, the muscle produces force while lengthening, the opposite occurs and muscle forces greater than the maximum isometric force are observed. Observing Figure 4.12, it can be concluded that

the maximum and minimum magnitude for force occurs during eccentric and concentric contractions, respectively. For eccentric contractions, a maximum force magnitude is reached, for which the force no longer increases regardless of the increase in lengthening velocity. The interval for the muscle contraction velocity is between $-v_0^m$ and $0.5v_0^m$, as observed in Figure 4.12, where the maximum contractile velocity, v_0^m , is approximately equal to ten times the muscle optimal length, $10l_0^m$ (Kaplan, 2000; Neumann, 2013; M. T. Silva, 2003; Yamaguchi, 2001).

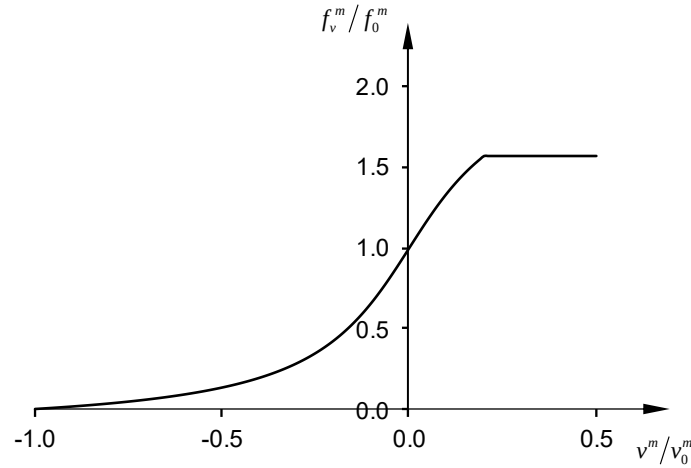


Figure 4.12 – Schematic representation of the force-velocity relation for the contractile element considering a fully activated muscle, i.e., $a=1$.

The condition for the force-velocity relation of the contractile element utilized in this work is based on approximation to experimental data reported by Kaplan (2000) and it is expressed as (Kaplan, 2000; M. T. Silva, 2003)

$$f_v^m = \begin{cases} 0 & v^m < -v_0^m \\ -\frac{f_0^m}{\arctan 5} \arctan\left(-5 \frac{v^m}{v_0^m}\right) + f_0^m & -v_0^m \leq v^m \leq 0.20v_0^m \\ \frac{\pi f_0^m}{4 \arctan 5} + f_0^m & v^m > 0.20v_0^m \end{cases} \quad (4.11)$$

where v^m is the muscle velocity and v_0^m denotes the maximum contractile velocity above which the muscle cannot produce force.

In this work, all muscle fibers are assumed to respond to the neural signal in the same manner (Yamaguchi, 2001) and, therefore, it is considered that the force-length and the force-velocity relations are linearly scaled by the muscle activation, as observed in Eq. (4.8). Figure 4.13 presents the force-length and force-velocity relations of the contractile element considering different levels of muscle activation.

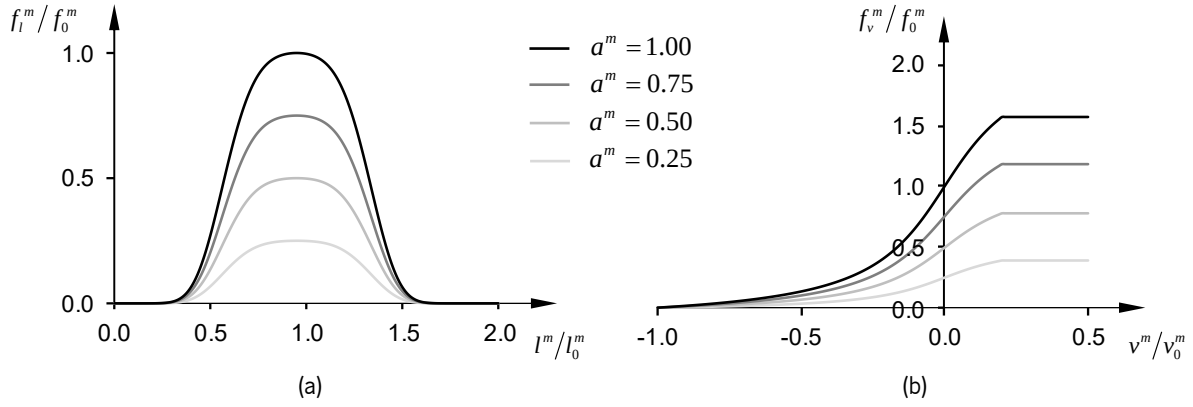


Figure 4.13 – Schematic representation of the (a) force-length and (b) force-velocity relation for the contractile element considering a different levels of muscle activation, a^m .

The force-length and force-velocity relations of the passive, Eq. (4.7), and contractile, Eq. (4.10) and Eq. (4.11), elements can be combined to construct the carpet plots presented in Figure 4.14.

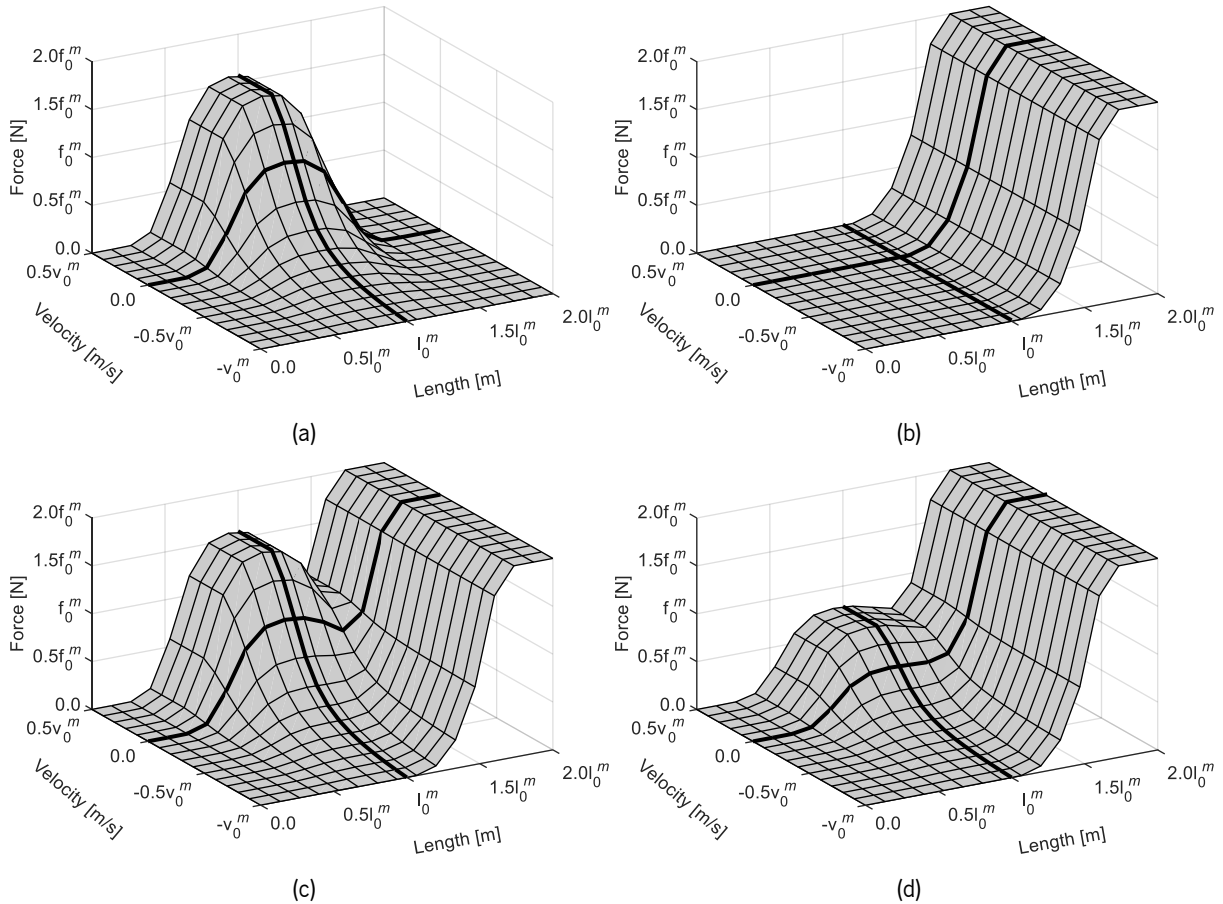


Figure 4.14 – Carpet plots of the force-length and force-velocity relations for the (a) contractile element, (b) passive element, (c) total muscle force with $a=1$, and (d) total muscle force with $a=0.5$.

The thick black lines in Figure 4.14 denote the force-length and force-velocity curves shown in Figure 4.9, Figure 4.10 and Figure 4.12. Although the force-length and force-velocity relations of the passive and contractile elements are described separately, in reality, they occur simultaneously during

muscular contraction. Observing Figure 4.14, it can be concluded that the force produced by the contractile element depends on the muscle length, velocity, and activation, while the force produced by the passive element is dependent on the muscle length only. It is also important to note that a muscle contracting at high velocities and short lengths produces relatively low force levels. In contrast, a muscle contracting at low velocities and at a longer length, is capable of producing substantially greater forces.

For Eqs.(4.7), (4.10) and (4.11), the muscle length and velocity must be determined. The muscle length can be determined by rearranging Eq. (4.2) as

$$l^m = \frac{l^{mtu} - l^t}{\cos \alpha} \quad (4.12)$$

In turn, the first time derivative of Eq. (4.2) yields the following condition

$$v^{mtu} = v^t + v^m \cos \alpha - l^m \sin \alpha \dot{\alpha} \quad (4.13)$$

where v^t represents the tendon velocity and $\dot{\alpha}$ denotes the pennation angular velocity, which is calculated by taking the first time derivative of Eq. (4.5) as

$$\dot{\alpha} = -\frac{v^m \sin \alpha}{l^m \cos \alpha} \quad (4.14)$$

It is important to note that Eq. (4.5) considers a constant relation between the muscle length and the pennation angle. For this assumption to be valid, the model must consider that all muscle fibers are parallel and equal in length, as stated previously.

Substituting Eq. (4.14) into Eq. (4.13), yields the expression for the MTU velocity, v^{mtu} , as

$$v^{mtu} = v^t + \frac{v^m}{\cos \alpha} \quad (4.15)$$

As explained in previous paragraphs, in this work, the tendon is assumed to be rigid, and, thus, the corresponding velocity is null. Hence, Eq. (4.15) can be updated to express the muscle velocity as

$$v^m = v^{mtu} \cos \alpha \quad (4.16)$$

Finally, taking into consideration Eqs. (4.6), (4.8) and (4.9), the total force produced by the MTU expressed in Eq. (4.3) can be rearranged as

$$f^{mtu} = \left(f_{PE}^m + \hat{f}_{CE}^m a^m \right) \cos \alpha = \left[f_{PE}^m + \left(\frac{f_l^m f_v^m}{f_0^m} \right) a^m \right] \cos \alpha \quad (4.17)$$

It should be noted that the expressions presented in Eqs. (4.7), (4.10) and (4.11) were taken from the works of Kaplan (2000) and M. T. Silva (2003), and can be substituted by others existing in the literature (Buchanan et al., 2004; Thelen, 2003; Winters, 1990).

4.3. Introduction of Muscles into the Equations of Motion

Skeletal muscles are introduced into the multibody models using muscle-tendon actuators, which are characterized by specifying their force generation properties, as explained in Section 4.2, and their geometry. Regarding this last issue, the MTUs are spatially defined by the coordinates of a series of points connected by line segments. The first and the last of these points correspond to the MTU origin (“o”) and insertion (“i”), respectively, while the remaining points represent the via-points (“v_p”). The consideration of via-points allows to define the geometry of the MTU more realistically (Oliveira et al., 2016; M. T. Silva, 2003). It is important to note that some geometrical assumptions are made, which do not correspond to the actual human anatomy, namely the MTUs have rectilinear orientations and constant cross-sectional area, and wrap around anatomical structures is not taken into consideration.

In this work, the skeletal MTUs are regarded to as forces which lines of action are defined by direction unit vectors, $\mathbf{u}_d$, as observed in Figure 4.15a. The direction unit vectors are utilized to define the orientation of the MTU forces in each muscle segment. Considering that a MTU develops a force of magnitude f^{mtu} , and taking into consideration Eq. (4.17), then the MTU force applied at a generic point with direction $\mathbf{u}_d$ can be expressed as

$$\mathbf{f}^{mtu} = \mathbf{u}_d f^{mtu} = \mathbf{u}_d \left(f_{PE}^m + \hat{f}_{CE}^m a^m \right) \cos \alpha = \mathbf{f}_{PE}^{mtu} + \hat{\mathbf{f}}_{CE}^{mtu} a^m \quad (4.18)$$

where the mathematical expressions for the forces of the passive and contractile elements projected onto the line of action of the tendon are, respectively, as

$$\mathbf{f}_{PE}^{mtu} = \mathbf{u}_d f_{PE}^m \cos \alpha \quad (4.19)$$

$$\hat{\mathbf{f}}_{CE}^{mtu} = \mathbf{u}_d \hat{f}_{CE}^m \cos \alpha \quad (4.20)$$

The number of direction unit vectors, n_u , is calculated using the following condition

$$n_u = n_{vp} + 1 \quad (4.21)$$

in which n_{vp} denotes the number of via-points utilized to define the MTU.

A MTU contains as many force application points as the number of points that are required to describe its structure. The total number of forces exerted in the application points, $n_{f^{mtu}}$, is given by

$$n_{f^{mtu}} = 2n_{vp} + 2 \quad (4.22)$$

A MTU with no via-points, that is, $n_{vp} = 0$, exerts a pair of forces at two application points, which represent the MTU origin and insertion, and thus, only one direction unit vector is required. In the simple biomechanical multibody system presented in Figure 4.15b, the number of force application points is

five, which correspond to the MTU origin, insertion and three via-points. A total of eight forces are exerted in these points, namely, one force is exerted at the MTU origin, one force is applied at the MTU insertion, and two forces are exerted in each via-point. In Figure 4.15, four direction unit vectors must be calculated. In addition, each point of force application is associated with a segment of the multibody system to which the MTU force is applied. For instance, the force $\mathbf{f}^{mtu,1}$ applied at the origin is associated with body 1. It is important to note that Figure 4.15 presents a simple example with no physiological meaning.

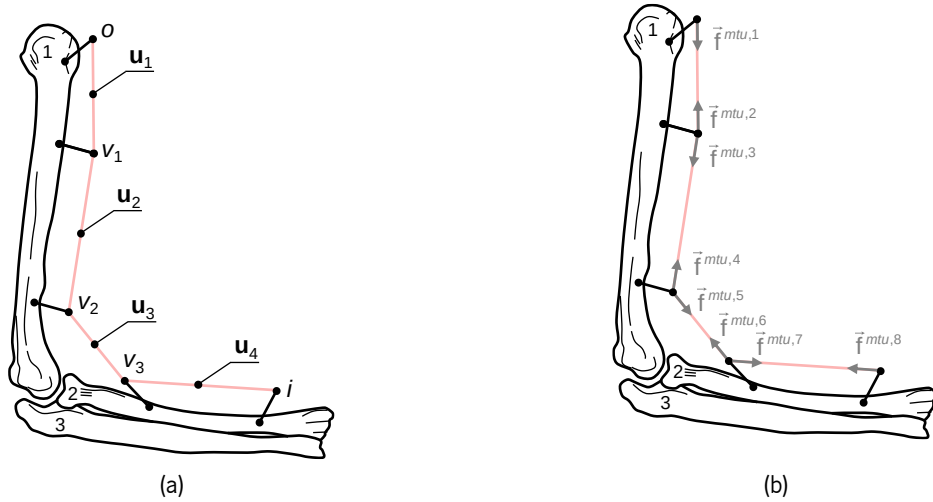


Figure 4.15 – Schematic representation of a simple three-segment biomechanical multibody system with a MTU defined by three via-points. Illustration of the (a) points of force application (o – origin, i – insertion and v_p – via-points, $p = 1, 2, 3$) and direction unit vectors, $\mathbf{u}_d$, $d = 1, 2, 3, 4$, and (b) MTU forces, $\mathbf{f}^{mtu}$, exerted at the application points.

The direction unit vectors, $\mathbf{u}_d$, are required for the calculation of the MTU length presented in Eq. (4.12) using the following condition

$$l^{mtu} = \sum_{d=1}^{n_p-1} \|\mathbf{u}_d\| = \sum_{d=1}^{n_p-1} \sqrt{\mathbf{u}_d^T \mathbf{u}_d} \quad (4.23)$$

where n_p is the total number of points defining the MTU and vector $\mathbf{u}_d$ is given by

$$\mathbf{u}_d = \mathbf{r}_j^{d+1} - \mathbf{r}_k^d \quad (4.24)$$

in which the subscripts j and k refer to the bodies to which the points $d+1$ and d belong, respectively. For example, for vector $\mathbf{u}_1$ of Figure 4.15a, the subscripts $d+1$ and d correspond to the first via-point, v_1 , and the origin, o , respectively. In this case, the subscripts j and k refer to the body 1 since both of these points are defined with respect to this body. The length of the MTU calculated using Eq. (4.23) varies according with the kinematics of the movement under analysis. In turn, the first time derivative of Eq. (4.23) yields the expression for the calculation of the MTU velocity required for Eq. (4.16) as

$$\mathbf{v}^{mtu} = \sum_{d=1}^{n_p-1} \frac{\mathbf{u}_d^T \dot{\mathbf{u}}_d}{\|\mathbf{u}_d\|} \quad (4.25)$$

where $\dot{\mathbf{u}}_d$ is calculated using the following condition

$$\dot{\mathbf{u}}_d = \dot{\mathbf{r}}_j^{d+1} - \dot{\mathbf{r}}_k^d \quad (4.26)$$

By considering the skeletal MTUs as external forces acting on the multibody system, the force magnitude is assumed to be the same at any point of the MTU and equal to the total force exerted by the MTU. For each muscle segment, the MTU force applied at each point of the segment is equal in magnitude but opposite in direction. For example, for the unit vector $\mathbf{u}_1$ of Figure 4.15 the following condition applies

$$\mathbf{f}^{mtu,2} = -\mathbf{f}^{mtu,1} \quad (4.27)$$

In order to integrate the MTU forces into the vector $\mathbf{g}$ of the equations of motion (3.14), they need to be transformed into a generalized force vector with respect to the entire system coordinates. For the biomechanical multibody system of Figure 4.15, vector $\mathbf{g}^{mtu}$, which represents the vector of generalized MTU forces and moments, is expressed as

$$\mathbf{g}^{mtu} = \begin{Bmatrix} \mathbf{f}_1^{mtu,1} + \mathbf{f}_1^{mtu,2} + \mathbf{f}_1^{mtu,3} + \mathbf{f}_1^{mtu,4} + \mathbf{f}_1^{mtu,5} \\ \mathbf{n}_1^{mtu,1} + \mathbf{n}_1^{mtu,2} + \mathbf{n}_1^{mtu,3} + \mathbf{n}_1^{mtu,4} + \mathbf{n}_1^{mtu,5} \\ \mathbf{f}_2^{mtu,6} + \mathbf{f}_2^{mtu,7} + \mathbf{f}_2^{mtu,8} \\ \mathbf{n}_2^{mtu,6} + \mathbf{n}_2^{mtu,7} + \mathbf{n}_2^{mtu,8} \\ \mathbf{0} \\ \mathbf{0} \end{Bmatrix} = \begin{Bmatrix} \mathbf{f}_1^{mtu,1} + \mathbf{f}_1^{mtu,2} + \mathbf{f}_1^{mtu,3} + \mathbf{f}_1^{mtu,4} + \mathbf{f}_1^{mtu,5} \\ \tilde{\mathbf{s}}_1^0 \mathbf{f}_1^{mtu,1} + \tilde{\mathbf{s}}_1^{v_1} \mathbf{f}_1^{mtu,2} + \tilde{\mathbf{s}}_1^{v_1} \mathbf{f}_1^{mtu,3} + \tilde{\mathbf{s}}_1^{v_2} \mathbf{f}_1^{mtu,4} + \tilde{\mathbf{s}}_1^{v_2} \mathbf{f}_1^{mtu,5} \\ \mathbf{f}_2^{mtu,6} + \mathbf{f}_2^{mtu,7} + \mathbf{f}_2^{mtu,8} \\ \tilde{\mathbf{s}}_2^{v_3} \mathbf{f}_2^{mtu,6} + \tilde{\mathbf{s}}_2^{v_3} \mathbf{f}_2^{mtu,7} + \tilde{\mathbf{s}}_2^i \mathbf{f}_2^{mtu,8} \\ \mathbf{0} \\ \mathbf{0} \end{Bmatrix} \quad (4.28)$$

where the first two rows are the generalized MTU forces and moments applied to body 1, rows three and four denote the generalized forces and moments applied to body 2, and the last two rows symbolize the generalized forces and moments applied to body 3. The muscle represented in Figure 4.15 does not have attachments points to body 3, which explains the fact that, in vector $\mathbf{g}^{mtu}$, the last two rows are null.

Equation (4.28) can be generalized for a multibody system with n_b bodies and n_{mtu} MTUs as

$$\mathbf{g}^{mtu} = \begin{Bmatrix} \sum_{n=1}^{n_{mtu}} \sum_{k=1}^{n_{f_{mtu}}} \mathbf{f}_1^{mtu,k} \\ \sum_{n=1}^{n_{mtu}} \sum_{k=1}^{n_{f_{mtu}}} \mathbf{n}_1^{mtu,k} \\ \dots \\ \dots \\ \sum_{n=1}^{n_{mtu}} \sum_{k=1}^{n_{f_{mtu}}} \mathbf{f}_{n_b}^{mtu,k} \\ \sum_{n=1}^{n_{mtu}} \sum_{k=1}^{n_{f_{mtu}}} \mathbf{n}_{n_b}^{mtu,k} \end{Bmatrix} \quad (4.29)$$

Taking advantage of the conditions expressed in Eqs. (4.18)-(4.20), it is possible to further develop Eq. (4.29) as

$$\mathbf{g}^{\text{mtu}} = \mathbf{g}_{\text{PE}}^{\text{mtu}} + \hat{\mathbf{g}}_{\text{CE}}^{\text{mtu}} \mathbf{a}^{\text{m}} = \begin{Bmatrix} \mathbf{f}_{\text{PE}}^{\text{mtu}} \\ \mathbf{n}_{\text{PE}}^{\text{mtu}} \end{Bmatrix} + \begin{Bmatrix} \hat{\mathbf{f}}_{\text{CE}}^{\text{mtu}} \\ \hat{\mathbf{n}}_{\text{CE}}^{\text{mtu}} \end{Bmatrix} \mathbf{a}^{\text{m}} \quad (4.30)$$

where $\mathbf{g}_{\text{PE}}^{\text{mtu}}$ is the vector of generalized forces and moments of the passive element projected onto the line of action of the tendon and $\hat{\mathbf{g}}_{\text{CE}}^{\text{mtu}}$ represents the vector of the generalized forces and moments of the available contractile element force projected onto the line of action of the tendon, which is multiplied by the muscle activation vector, $\mathbf{a}^{\text{m}}$, expressed as

$$\mathbf{a}^{\text{m}} = \begin{Bmatrix} a^1 \\ \dots \\ a^{n_m} \end{Bmatrix} \quad (4.31)$$

where n_m denotes the number of muscles composing the multibody system.

The vector of external generalized forces and gyroscopic moments, $\mathbf{g}$, of Eq. (3.14) can now be updated to include the muscle forces and moments of Eq. (4.30) acting on a multibody system

$$\mathbf{g} = \mathbf{g}^{\text{ext}} + \mathbf{g}^{\text{mtu}} = \mathbf{g}^{\text{ext}} + \mathbf{g}_{\text{PE}}^{\text{mtu}} + \hat{\mathbf{g}}_{\text{CE}}^{\text{mtu}} \mathbf{a}^{\text{m}} \quad (4.32)$$

in which $\mathbf{g}^{\text{ext}}$ is the vector of the remaining external generalized forces and moments acting on the system, such as the gravitational force and the foot-ground reaction forces.

The updated vector $\mathbf{g}$ can be incorporated into the first branch of Eq. (3.14), yielding

$$\mathbf{M}\dot{\mathbf{v}} + \mathbf{D}^T \boldsymbol{\lambda} = \mathbf{g}^{\text{ext}} + \mathbf{g}_{\text{PE}}^{\text{mtu}} + \hat{\mathbf{g}}_{\text{CE}}^{\text{mtu}} \mathbf{a}^{\text{m}} \quad (4.33)$$

The solution of Eq. (4.33) includes the vector of the Lagrange multipliers, $\boldsymbol{\lambda}$, and the muscle activations vector, $\mathbf{a}^{\text{m}}$. Rearranging Eq. (4.33) to organize the unknown and known quantities on the left and right sides of the equation, respectively, results in the following condition

$$\mathbf{D}^T \boldsymbol{\lambda} - \hat{\mathbf{g}}_{\text{CE}}^{\text{mtu}} \mathbf{a}^{\text{m}} = \mathbf{g}^{\text{ext}} + \mathbf{g}_{\text{PE}}^{\text{mtu}} - \mathbf{M}\dot{\mathbf{v}} \quad (4.34)$$

Expressing Eq. (4.34) in matrix terms yields

$$\begin{bmatrix} \mathbf{D}^T & -\boldsymbol{\chi}^T \end{bmatrix} \begin{Bmatrix} \boldsymbol{\lambda} \\ \mathbf{a}^{\text{m}} \end{Bmatrix} = \mathbf{g}^{\text{ext}} + \mathbf{g}_{\text{PE}}^{\text{mtu}} - \mathbf{M}\dot{\mathbf{v}} \quad (4.35)$$

where vector $\boldsymbol{\chi}$ is expressed as

$$\boldsymbol{\chi} = \begin{bmatrix} \hat{\mathbf{g}}_{\text{CE}}^1 & \dots & \hat{\mathbf{g}}_{\text{CE}}^{n_{\text{mtu}}} \end{bmatrix}^T \quad (4.36)$$

4.4. Optimization Procedure

The final configuration of the equations of motion (4.33) includes the MTU as external forces acting on the multibody system, resulting in a system with n_c constraint equations and $(n_\lambda + n_a)$ unknowns, in which n_λ represents the number of Lagrange multipliers and n_a denotes the number of muscle activations. Since $n_c < (n_\lambda + n_a)$, the system has an infinite number of solutions, a fact that can be physiologically understood as the existence of muscle redundancy. In complex biomechanical systems, the joints are crossed by several muscles, which means that different muscle activation patterns can generate the same movement or posture of the human body. It is the central nervous system that is responsible for selecting one of those multiple combinations and activating the muscles that best fulfill specific physiological criteria, depending on the task being performed and/or the objectives to be achieved. Mathematically, the muscle redundancy problem results from the fact that the number of muscle activations exceeds the number of degrees-of-freedom of the model and, thus, a unique solution for the analytical determination of the muscle forces cannot be obtained. Hence, the solution for indeterminate problems can be found through the use of appropriate optimization procedures, which estimate the optimal muscle activations according with the minimization of cost functions that simulate the decisions taken by the central nervous system when executing a certain task. Besides ensuring the minimization of the chosen cost function, the optimal solution must also satisfy the equations of motion of the model (Oliveira et al., 2016; M. T. Silva, 2003).

From a mathematical point of view, a generic optimization problem can be formulated as (Boyd & Vandenberghe, 2004)

$$\begin{aligned}
 \text{Given:} \quad & \mathbf{x} = \{x_i\} & i = 1, \dots, n_{dv} \\
 \text{Minimize:} \quad & \mathfrak{F}_0(\mathbf{x}) \\
 \text{Subject to:} \quad & \begin{cases} f_j(\mathbf{x}) = 0 & j = 1, \dots, n_{ec} \\ f_j(\mathbf{x}) \geq 0 & j = (n_{ec} + 1), \dots, n_{tc} \\ x_i^{\text{lower}} \leq x_i \leq x_i^{\text{upper}} \end{cases}
 \end{aligned} \tag{4.37}$$

where $\mathbf{x}$ is the vector of the design variables x_i , $\mathfrak{F}_0(\mathbf{x})$ represents the cost function to be minimized, and $f_i(\mathbf{x})$ and $f_j(\mathbf{x})$ denotes the constraint equations to which the control variables are subjected. There is total of n_{dv} design variables, which are bounded between x_i^{lower} and x_i^{upper} using side constraints. From the total n_{tc} constraint equations, n_{ec} are from equality type and $n_{tc} - n_{ec}$ are from inequality type. A vector $\mathbf{x}$ is considered optimal if it exhibits the minimal objective value among all vectors that satisfy the optimization constraints.

In this work, a static optimization procedure is employed, in which each MTU is considered to be an instantaneously available actuator which corresponding force is dependent on the current activation level only. Consequently, the optimization can be carried out independently at each time instant (Quental, 2013). Since static optimization only accounts for instantaneous performance criteria, it may not be capable of simulating accurately the actual behavior of the central nervous system when selecting a muscle activation set for a certain task (Ackermann, 2007). In turn, dynamic optimization is associated with high computational times, which is a disadvantage for the analysis of complex systems. However, as concluded by F. C. Anderson & Pandy (2001), static optimization is adequate for analyzing human gait.

In this work, the vector of the design variables comprises the vector of the Lagrange multipliers associated with all constraint equations of the system, as well as the vector of the muscle activations as

$$\mathbf{x} = \{\boldsymbol{\lambda} \quad \mathbf{a}^m\}^T \quad (4.38)$$

The solution of Eq. (4.38) is, however, subjected to the constraints associated with the multibody model. An important constraint equation is the one imposed by the equations of motion of the system. Hence, at each instant of time, the musculoskeletal model must satisfy the following equality condition

$$\mathbf{f}_{eq} = \begin{bmatrix} \mathbf{D}^T & -\boldsymbol{\chi}^T \end{bmatrix} \begin{Bmatrix} \boldsymbol{\lambda} \\ \mathbf{a}^m \end{Bmatrix} - (\mathbf{g}^{ext} + \mathbf{g}_{PE}^{mtu} - \mathbf{M}\dot{\mathbf{v}}) = \mathbf{0} \quad (4.39)$$

When considering a biomechanical multibody model without muscles, the Lagrange multipliers associated with the rotational driving constraints of the system translate the contributions of the joint drivers to the prescribed movement. However, when muscles are incorporated into the model, the main objective is to determine their contributions to the movement under analysis. In this situation, it is intended that the rotational driver contributions are minimized and that the muscles are the only structures responsible for the movement of the model, thus, mimicking what actually occurs during human motion. In this work, the Lagrange multipliers associated with the rotational driving constraints of the joints spanned by the muscles are forced to values close to zero during the optimization procedure, which allows for an intuitive manner of estimating the muscle activations. Hence, to guarantee the fulfillment of the equality constraint (4.39), the muscle activations from the optimization must compensate for this situation and the following inequality constraint must be considered (A. Pereira et al., 2011)

$$-\varepsilon \leq \boldsymbol{\lambda}^* \leq \varepsilon \quad (4.40)$$

where $\boldsymbol{\lambda}^*$ represents the vector of the Lagrange multipliers associated with the rotational driving constraints of the joints spanned by the muscles and ε is a user-specified tolerance that must be small enough in order to ensure that the rotational driver contributions are disregarded. The Lagrange multipliers included in vector $\boldsymbol{\lambda}^*$ are those associated with Eqs.(3.82)-(3.121).

The remaining Lagrange multipliers, that is, those associated with the joint constraints and the rigid body driving constraints can assume any value, resulting in

$$-\infty < \boldsymbol{\lambda}^R < +\infty \quad (4.41)$$

in which $\boldsymbol{\lambda}^R$ denotes the vector of the Lagrange multipliers associated with the joint constraints and the rigid body driving constraints. For the rigid body driving constraints, the Lagrange multipliers included in vector $\boldsymbol{\lambda}^R$ are those associated with Eqs.(3.67)-(3.81).

Finally, the muscle activations, a^m , must always be positive and bounded between 0 and 1 in order to ensure the optimization procedure returns values within physiological limits. The corresponding side constraint can be expressed as

$$0 \leq a^m \leq 1 \quad (4.42)$$

In summary, the general optimization procedure considered in this work is described as

$$\begin{aligned} \text{Given:} \quad & \mathbf{x} = \left\{ \boldsymbol{\lambda} \quad \mathbf{a}^m \right\}^T \\ \text{Minimize:} \quad & \mathfrak{F}_0(\mathbf{x}) \\ \text{Subject to:} \quad & \begin{cases} \mathbf{f}_{\text{eq}} = \begin{bmatrix} \mathbf{D}^T & -\boldsymbol{\chi}^T \end{bmatrix} \begin{Bmatrix} \boldsymbol{\lambda} \\ \mathbf{a}^m \end{Bmatrix} - (\mathbf{g}^{\text{ext}} + \mathbf{g}_{\text{PE}}^{\text{mtu}} - \mathbf{M}\dot{\mathbf{v}}) = \mathbf{0} \\ 0 \leq a^m \leq 1 \\ -\varepsilon \leq \boldsymbol{\lambda}^* \leq \varepsilon \\ -\infty < \boldsymbol{\lambda}^R < +\infty \end{cases} \end{aligned} \quad (4.43)$$

In biomechanics of motion, there are several types of cost functions responsible for simulating the physiological criteria adopted by the central nervous system when choosing which muscles should be recruited and with which level of activation in order to produce adequate motion or posture for the tasks under analysis. It is important to note that the selection of the most appropriate cost function to utilize in the optimization procedure relies on several aspects, such as the type of movement under investigation, the objectives to be achieved or the presence of pathological conditions (M. T. Silva, 2003). The cost functions considered in this work are the following

(i) Sum of the square of the muscle activations

The objective of this cost function is to minimize the muscle activations, which, in turn, represents the minimization of the neural effort required for the execution of a motor task. The expression utilized for this cost function is as

$$\mathfrak{F}_0 = \sum_{m=1}^{n_m} (a^m)^2 \quad (4.44)$$

(ii) Sum of the square of the individual contractile element forces

This cost function was proposed for applications of the human locomotion and its purpose is to minimize the energy consumption. The expression considered for the minimization of the sum of the square of the muscle activations is the following

$$\mathfrak{J}_0 = \sum_{m=1}^{n_m} (f_{CE}^m)^2 = \sum_{m=1}^{n_m} \left(\frac{f_l^m f_v^m}{f_0^m} a^m \right)^2 \quad (4.45)$$

(iii) Sum of the cube of the individual average muscle stresses

The last cost function was introduced by Crowninshield & Brand (1981) and its purpose is to minimize the energy consumption. An important aspect is that the function accounts for physiological information of each muscle, namely the physiological cross-sectional area. The considered expression is as

$$\mathfrak{J}_0 = \sum_{m=1}^{n_m} (\sigma_{CE}^m)^3 = \sum_{m=1}^{n_m} \left(\bar{\sigma} \frac{f_l^m f_v^m}{(f_0^m)^2} a^m \right)^3 \quad (4.46)$$

in which $\bar{\sigma}$ represents the specific muscle strength, which has a constant value of 31.39 N/cm² (Yamaguchi, 2001).

In this work, the gradients of each cost function were also utilized in the optimization procedure in order to obtain faster computations by using the gradient information of the objective function during iterations. Mathematically, the gradient of the cost function at a point consists of a vector containing the partial derivatives of $\mathfrak{J}_0(\mathbf{x})$ with respect to each design variable. The gradient vector at a certain point points in the direction of the maximum increase in the cost function at that point. Hence, the direction of maximum decrease is opposite to that, that is, negative of the gradient vector. The negative gradient vector, thus, denotes a direction of steepest descent for the cost function, which is the goal in optimization procedures (Arora, 1989; Garzelli et al., 2008; Jin et al., 2019). For the particular case of this work, the general form of the gradient vector is expressed as

$$\nabla \mathfrak{J}_0 = \left\{ \frac{\partial \mathfrak{J}_0}{\partial \boldsymbol{\lambda}} \quad \frac{\partial \mathfrak{J}_0}{\partial \mathbf{a}^m} \right\}^T \quad (4.47)$$

In Eq. (4.47), each partial derivative represents the rate of instantaneous change of the cost function in the direction of each respective design variable. It is important to note that the cost functions (4.44)-(4.46) are not dependent on vector $\boldsymbol{\lambda}$, and, therefore, the gradient of the cost function becomes

$$\nabla \mathfrak{J}_0 = \left\{ \frac{\partial \mathfrak{J}_0}{\partial \mathbf{a}^m} \right\}^T \quad (4.48)$$

The gradients for the cost functions (4.44), (4.45) and (4.46) can be obtained analytically using Eq. (4.48) and are expressed, respectively, as

$$\nabla \mathfrak{S}_0 = \{2\mathbf{a}^m\}^T \quad (4.49)$$

$$\nabla \mathfrak{S}_0 = \left\{ 2 \left(\frac{f_l^m f_v^m}{f_0^m} \right)^2 \mathbf{a}^m \right\}^T \quad (4.50)$$

$$\nabla \mathfrak{S}_0 = \left\{ 3 \left(\frac{f_l^m f_v^m}{(f_0^m)^2} \right)^3 (\mathbf{a}^m)^2 \right\}^T \quad (4.51)$$

4.5. Application Examples

In the present section, two examples of application are considered. The first example involves an antagonistic muscle pair, in which the MTUs are modeled either with origin and insertion only, or with origin, insertion and one via-point. The purpose of this first analysis is to validate the skeletal muscle modeling methodology discussed throughout this chapter. Then, the second application example presents a more realistic case scenario. The aim is to extend to investigation presented in section 3.5.1, in which the ankle joint complex was formulated as a modified universal joint, to incorporate the muscle behavior.

4.5.1. Application Example 1: Antagonist Muscle Action

In this application example, a double pendulum multibody model is considered and implemented in MUBODYNA. The two rigid bodies of the system, designated as bars 1 and 2, are assumed to be solid cylinders with 0.025 m of radius. The two bodies are kinematically connected to each other using one revolute joint, which allows motion in the xz plane around the y axis. The translation and orientation of bar 1 are constrained. Hence, the model has one degree-of-freedom. The local coordinate systems of each body are located at their center of mass (see Figure 4.16) and are aligned with the principal axes of inertia. The initial configuration of the double pendulum multibody model is illustrated in Figure 4.16 and the corresponding initial conditions are presented in Table 4.1.

Table 4.1 – Initial conditions for the double pendulum multibody model

Body (nr.)	x [m]	y [m]	z [m]	e_1	e_2	e_3	e_4
Bar 1 (1)	0.0000	0.0000	-0.5000	1.0000	0.0000	0.0000	0.0000
Bar 2 (2)	0.0000	0.0000	-1.5000	1.0000	0.0000	0.0000	0.0000

The dimensions and inertial properties of the double pendulum are listed in Table 4.2.

Table 4.2 – Dimensions and inertial properties of the bodies of the double pendulum multibody model

Body (nr.)	Length [m]	Mass [kg]	Moment of inertia [kg·m ²]		
			$I_{\xi\xi}$	$I_{\eta\eta}$	$I_{\zeta\zeta}$
Bar 1 (1)	1.0000	1.0000	0.0833333	0.0833333	0.0003125
Bar 2 (2)	1.0000	1.0000	0.0833333	0.0833333	0.0003125

The simulation parameters utilized in all dynamic simulations are displayed in Table 3.4. The simulation time is considered to be 2.00 seconds.

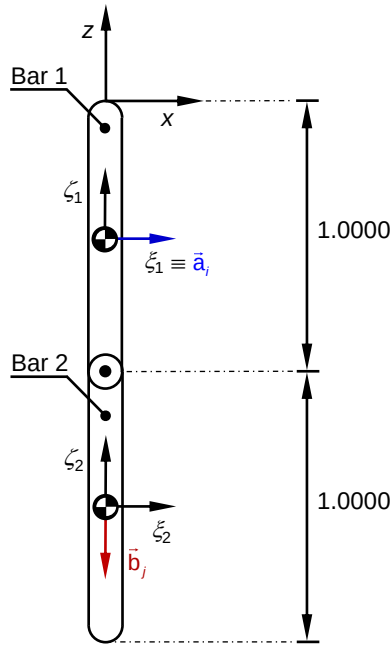


Figure 4.16 – Schematic representation of the double pendulum multibody model.

A rotational driving constraint similar to Eq. (3.82) is provided to the multibody model in order to guide the revolute joint angle. The function utilized to prescribe the joint angle is as (see Figure 4.17)

$$\theta^*(t) = \frac{\pi}{2} - \frac{\pi}{6} \sin(\pi t) \quad (4.52)$$

In this case, the $\mathbf{a}_i$ and $\mathbf{b}_j$ vectors of Eq. (3.82) are defined, respectively, as (see Figure 4.16)

$$\mathbf{a}_i = [1 \quad 0 \quad 0]^T \quad (4.53)$$

$$\mathbf{b}_j = [0 \quad 0 \quad -1]^T \quad (4.54)$$

where bodies i and j are bar 1 and bar 2, respectively.

It is important to note that, due to the application of Eq. (4.52) for the rotational driving constraint (3.82), the initial linear and angular velocities of bar 2 are different from zero. However, since bar 1 is fixed to the ground, its initial velocities are null. The gravitational force acts on the negative z direction.

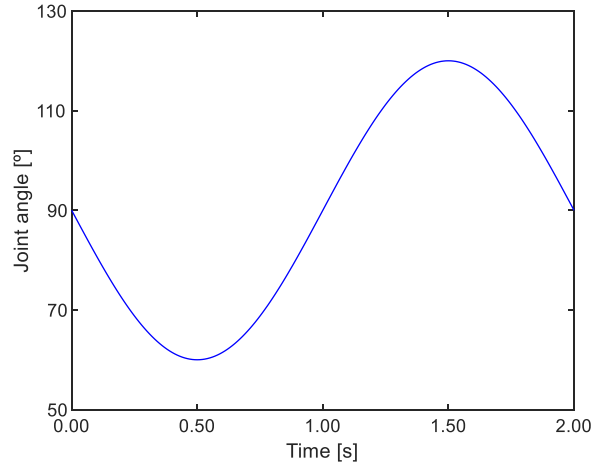


Figure 4.17 – Rotational driving constraint utilized the guide the revolute joint angle of the double pendulum model.

Figure 4.18 shows several snapshots of the movement of the double pendulum multibody model, which is guided using Eq. (4.52) and the plot presented in Figure 4.17, during the 2-second simulation.

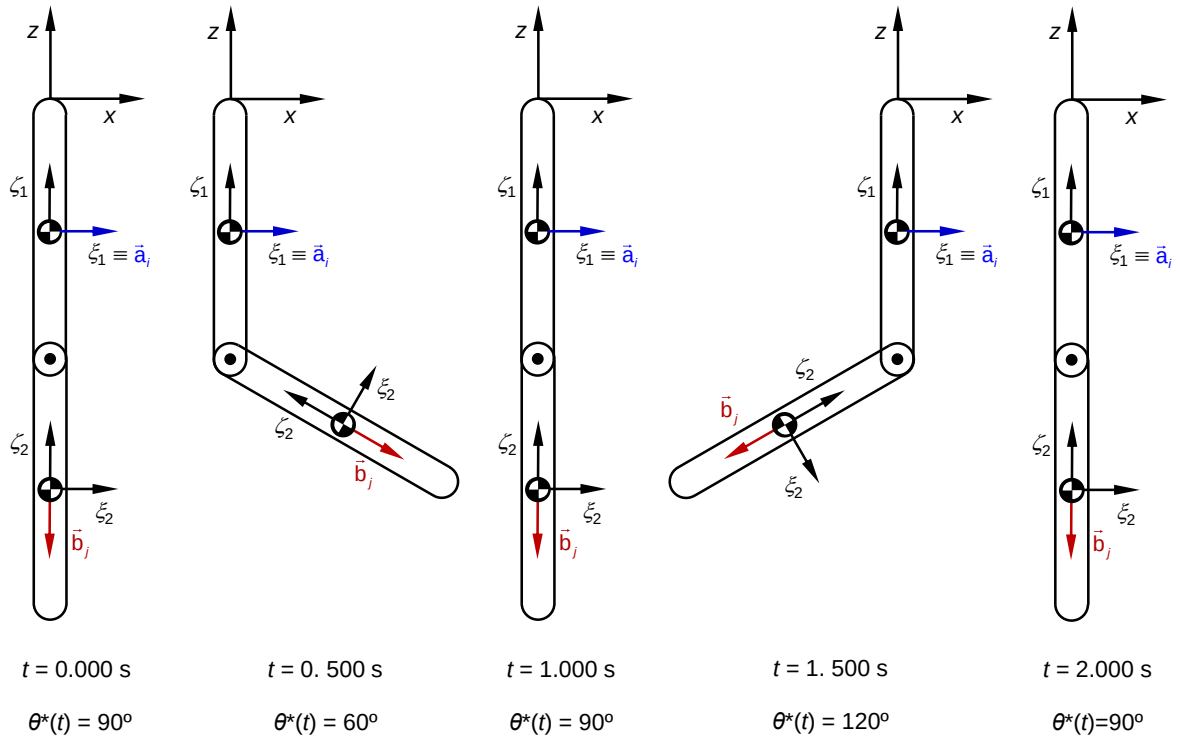


Figure 4.18 – Snapshots of the movement of the double pendulum multibody model for the 2-second simulation.

An antagonist muscle pair is considered, in which the MTUs are modeled either using origin and insertion only (see Figure 4.19a), or using origin, insertion and one via-point (see Figure 4.19b). In Figure 4.19, the MTU located on the side of the positive x -axis is considered to be the flexor, while the MTU located on the negative x -axis side is the extensor. The maximum isometric muscle force, f_0^m , and the optimal muscle pennation angle, α_0 , have the same values of 100 N and 10° , respectively, for both models and for all muscles. In addition, in this example, the length of the MTU, l^{mtu} , was established as 1.10 m and

1.05 m for the flexor and the extensor MTU, respectively. Hence, the length of the muscle, l^m , and the tendon length, l^t , were calculated, respectively, as

$$l^m = 0.25l^{mtu} \quad (4.55)$$

$$l^t = 0.75l^{mtu} \quad (4.56)$$

Table 4.3 depicts the MTU parameters utilized for both the model without and with one via-point.

Table 4.3 – Parameters utilized for the MTUs considered in the double pendulum multibody model

	MTU name	Body name	Point name	Local coordinates of the points [m]		
				ξ	η	ζ
Model without via-points	Flexor	Bar 1	Origin	0.075	0.000	0.500
		Bar 2	Insertion	0.075	0.000	0.400
	Extensor	Bar 1	Origin	-0.100	0.000	0.500
		Bar 2	Insertion	-0.100	0.000	0.450
Model with one via-point	Flexor	Bar 1	Origin	0.075	0.000	0.500
		Bar 1	Via-point	0.075	0.000	-0.500
		Bar 2	Insertion	0.025	0.000	0.400
	Extensor	Bar 1	Origin	-0.100	0.000	0.500
		Bar 1	Via-point	-0.100	0.000	-0.450
		Bar 2	Insertion	-0.050	0.000	0.450

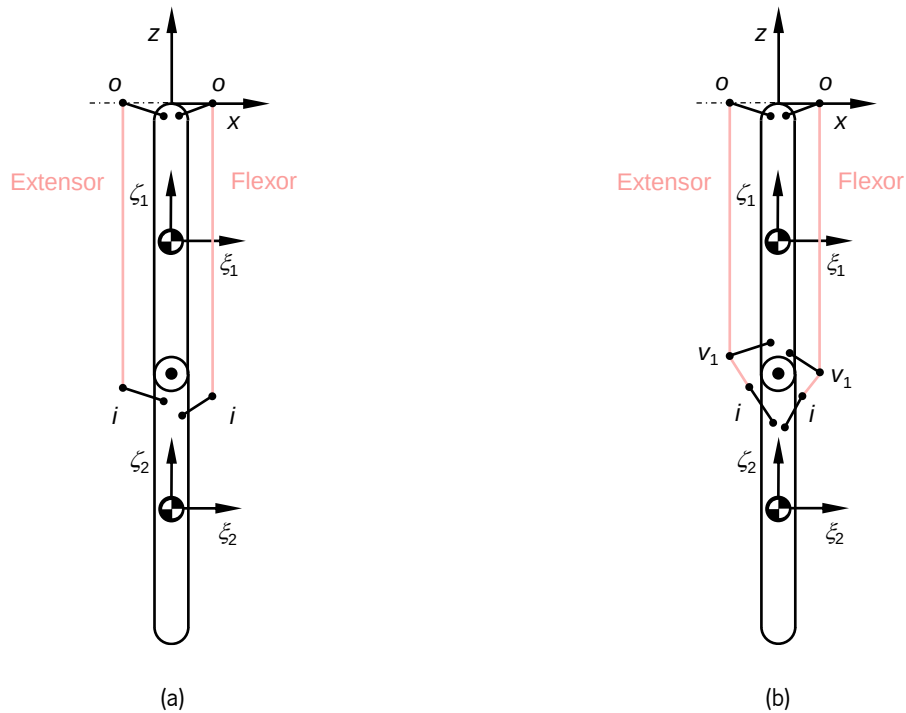


Figure 4.19 – Schematic representation of the double pendulum multibody model with muscles. Model (a) without via-points and (b) with one via-point. The subscripts o , i and v_1 represent the MTU origin, insertion and via-point, respectively.

The optimization procedure described in section 4.4 was applied to find the muscle activation patterns using Eqs. (4.44)-(4.46). In Eq. (4.40), ε was set to 10^{-15} . Since the multibody model is very simple, the application of distinct cost functions produces no significantly different muscle activation patterns (see Appendix C). Hence, Figure 4.20 depicts the results obtained using Eq. (4.46) only. For both models, the optimization procedure converged to a solution in which the activation of the flexor MTU is not null from 0.00 s to 1.00 s of simulation in order to pull bar 2 anticlockwise and allow flexion of the revolute joint (see Figure 4.18). During this period of time, the activation of the extensor MTU is null (see Figure 4.20a and Figure 4.20b). As observed in Figure 4.20c and Figure 4.20d, during this period, both the flexor and the extensor MTUs produce force. The force of the flexor MTU is exclusively associated with the force produced by the contractile element, due to the fact that the muscle activation is not null and the muscle length is less than its optimal length, which means that the passive element is not capable of producing force. In turn, the force of the extensor MTU is exclusively associated with the force produced by the passive element, since the muscle activation is null and the normalized muscle length exhibits values that exceed 1.00, meaning that the muscle is stretched beyond its optimal length (see Figure 4.20e and Figure 4.20f). When the direction of the driving constraint is inverted at 1.00 s of simulation (see Figure 4.17), the extensor MTU is active in order to pull the bar 2 clockwise and allow revolute joint extension, while the activation of the flexor MTU is null (see Figure 4.20a and Figure 4.20b). Regarding the MTU forces, similar conclusions as the ones drawn from 0.00 s to 1.00 s can now be drawn for the simulation time from 1.00 s to 2.00 s. In this situation, the force of the flexor MTU is exclusively due to the action of the passive element due to the fact the muscle activation is null and the normalized muscle length is greater than 1.00. In turn, the extensor MTU force is only related to the force produced by the contractile element, since the muscle activation is not null and the muscle length is shorter than the optimal length (see Figure 4.20e and Figure 4.20f).

From the detailed analysis of the previous paragraph, it can be concluded that the antagonist behavior of the flexor and extensor MTUs is clear, as they are active in alternate periods throughout the simulation. In addition, it can be observed that the muscle activations and the MTU forces for the model with one via-point are higher than those obtained for the model without via-points. This phenomenon is related to the differences in the geometry of the MTUs in both models, which, in turn, is associated with the ability of the muscle to produce force. In the model without via-points, the muscle segment between the origin and the insertion is responsible for moving bar 2, while in the model with one via-point, the movement of bar 2 is due to the muscle segment between the via-point and the insertion (see Figure 4.19). It is, thus, clear that the muscle segment responsible for producing force is shorter in the model with one via-point, forcing the optimizer to converge to a solution in which the optimal muscle activations are greater.

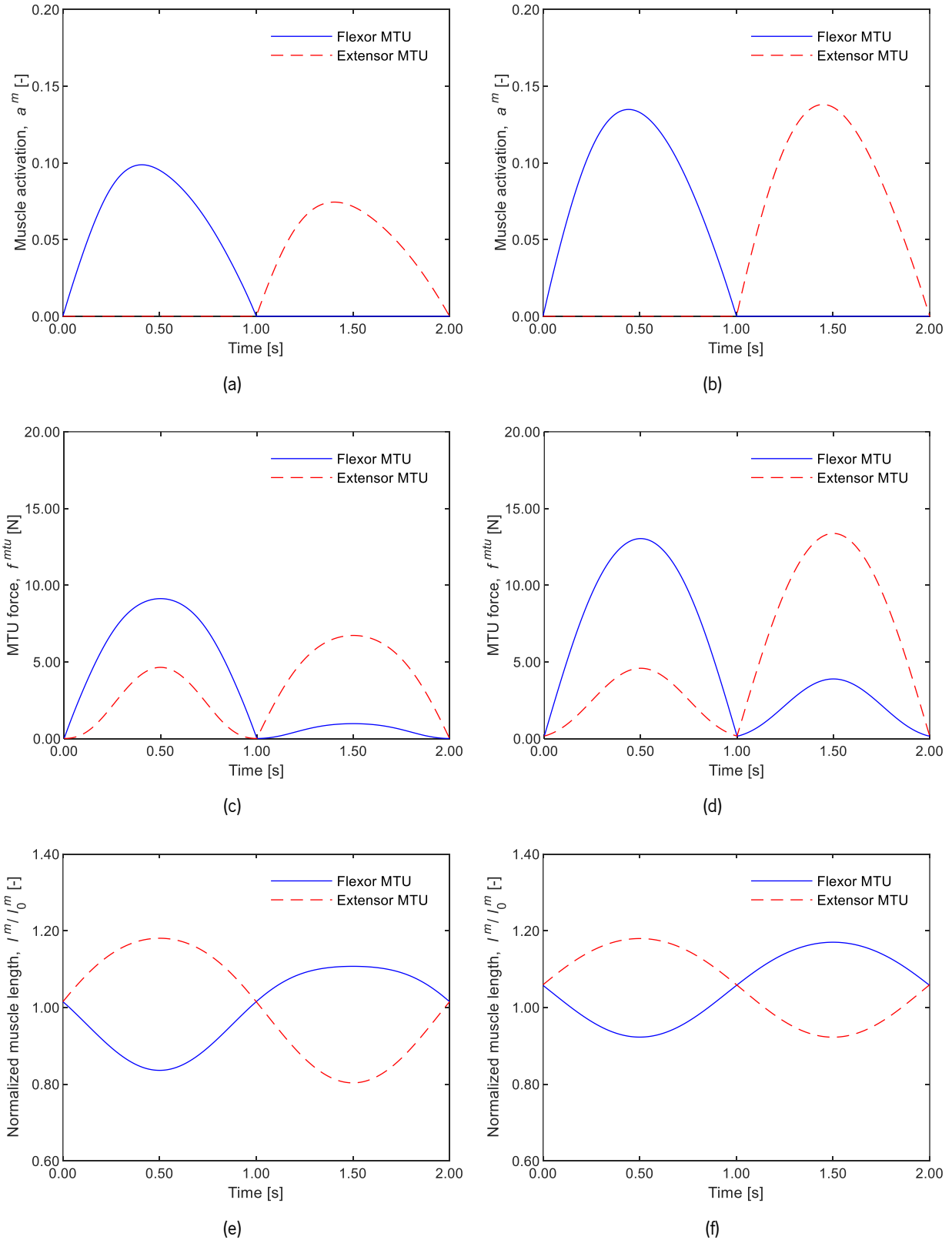


Figure 4.20 – Muscle activation, a^m , for the model (a) without and (b) with one via-point. Force of the MTU, f^{mtu} , for the model (c) without and (d) with one via-point. Normalized muscle length, l^m/l_0^m , for the model (e) without and (f) with one via-point.

The carpet plots presented in Figure 4.14 have been applied to this specific example of application and are utilized to analyze the force-generating capacity of the flexor and extensor MTUs, as

observed in Figure 4.21. The thick blue and red lines represent the force-length and force-velocity relations associated with the flexor and extensor MTUs, respectively. Observing Figure 4.21, it can be concluded that, for both models, the MTUs are working in the ideal force-generating zone, which means that the muscle length varies around the optimal length and the muscle velocity varies around zero. Thus, taking into consideration Figure 4.10 and Figure 4.12, both MTUs are capable of producing forces close to the maximum isometric force. In addition, both MTUs work on the concentric and eccentric contraction zones.

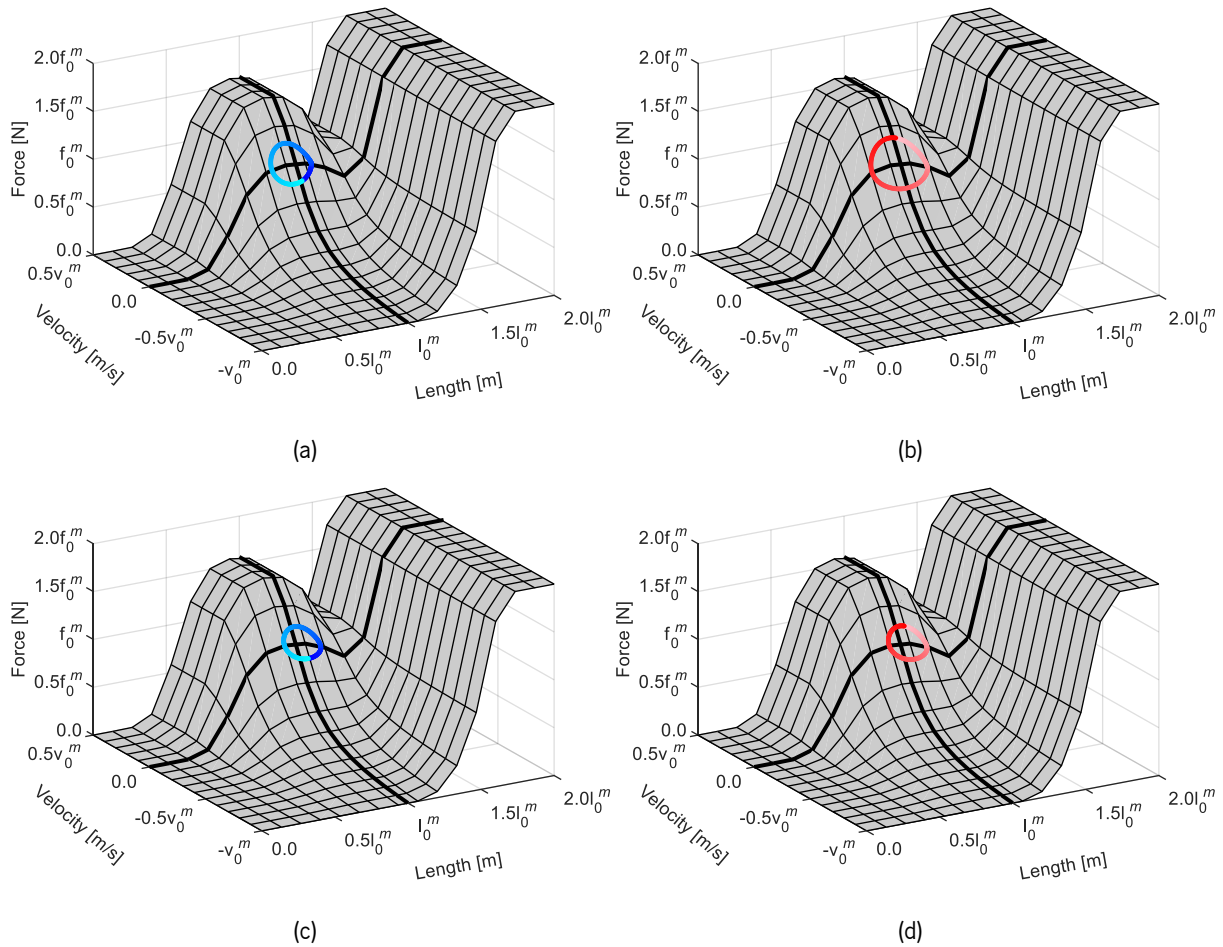


Figure 4.21 – Carpet plots for the (a, c) flexor and (b, d) extensor MTUs, assuming full muscle activation, that is, $a^m = 1$. The plots (a) and (b) refer to the model without via-points, and the plots (c) and (d) refer to the model with one via-point. The color of the plots vary from light to dark blue or red, which represents the beginning and end of the simulation, respectively.

From the conclusions drawn from the analysis of Figure 4.20 and Figure 4.21, it can be established that the implemented muscle modeling methodology is validated and is producing expected results. Other relevant results that further validate the methodology can be consulted in Appendix C.

This first example was selected in order to validate and demonstrate the application of the muscle modeling procedures described in this chapter due to its simplicity and resemblance to the physiological muscle action that occurs in the human body. However, it is important to note that the considered values for the parameters of the MTUs do not have physiological relevance.

4.5.2. Application Example 2: Ankle Joint Complex with Muscles

In this section, the three-dimensional biomechanical multibody model presented in section 3.5.3. is utilized. However, the pelvis segment is disregarded. The model is extended to include the muscles responsible for controlling the movements of the ankle joint complex of the human foot, with the purpose of analyzing a more realistic scenario. The anthropometric data, the bodies' local coordinate systems and location of the joints with respect to the local coordinate system of each body are defined in Chapter 5.

The biomechanical model is composed of four rigid bodies, namely, the thigh, leg, main foot and toes, which are connected to each other using three joints, namely the knee, ankle complex and metatarsophalangeal joints. The knee and the metatarsophalangeal joints are formulated as revolute joints, while the ankle joint complex is considered as a modified universal joint. The resulting multibody model has 10 degrees-of-freedom, which correspond to the flexion/extension of the toes, inversion/eversion of the main foot, plantarflexion/dorsiflexion of the main foot and flexion/extension of the leg. The remaining six degrees-of-freedom represent the translation and rotation of the biomechanical multibody model as a whole. The designation of the bodies and joints, as well as the location of the centers of mass of each body can be consulted in Figure 4.22a.

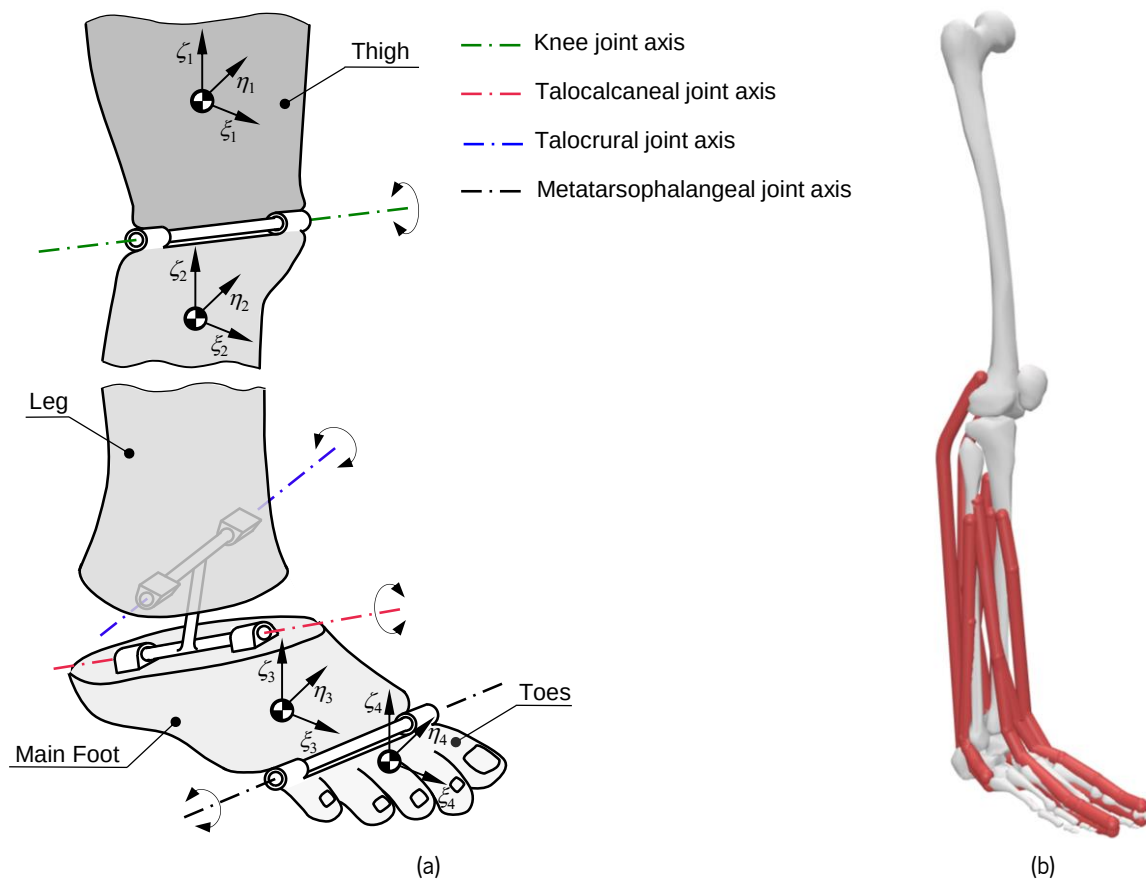


Figure 4.22 – Schematic representation of the biomechanical multibody model of the human thigh, leg, main foot and toes (a) without and (b) with muscles.

In this work, eleven muscles that control the two degrees-of-freedom of the ankle joint complex are considered and added to the model (see Figure 4.22b). The designation of each muscle, as well as a description of the action performed in the ankle complex is provided in Table 4.4. The physiological and geometric properties of the muscles considered in this example can be consulted in Appendix D.

Table 4.4 – Designation and action in the ankle complex of the muscles considered in the biomechanical multibody model

Muscle designation	Action	Muscle designation	Action
Soleus	Plantarflexion	Flexor Hallucis Longus	Plantarflexion; Inversion
Gastrocnemius Lateral Head	Plantarflexion	Extensor Digitorum Longus	Dorsiflexion; Eversion
Gastrocnemius Medial Head	Plantarflexion	Extensor Hallucis Longus	Dorsiflexion; Inversion
Tibialis Posterior	Plantarflexion; Inversion	Peroneus Brevis	Plantarflexion; Eversion
Tibialis Anterior	Dorsiflexion; Inversion	Peroneus Longus	Plantarflexion; Eversion
Flexor Digitorum Longus	Plantarflexion; Inversion		

Since the number of muscles (11) exceeds the number of degrees-of-freedom associated with the ankle joint complex (2), the muscle redundancy problem arises. Hence, a unique solution for the analytical determination of the muscle forces cannot be obtained and the optimization procedure described in section 4.4. must be applied. It is important to note that the thigh was added because the medial and lateral heads of the gastrocnemius have origin in this body (see Appendix D). The addition of the thigh implies the consideration of the knee joint, which, in turn, implies the inclusion of the muscles responsible for controlling this degree-of-freedom. However, the purpose of this section is to analyze the muscles that control the movements of the ankle joint complex. Thus, in this example of application, the knee joint is guided using the rotational driving constraint of Eq. (3.82), and the Lagrange multiplier associated with this kinematic constraint is unbounded using values of $\pm 10^9$ in Eq. (4.41) of the optimization. The Lagrange multipliers related to the driving constraints for the talocrural, talocalcaneal and metatarsophalangeal joints are bounded using a value of $\pm 10^2$ for ε in Eq. (4.40). The remaining Lagrange multipliers are unbounded with $\pm 10^9$, and the muscle activations are bounded using Eq. (4.42).

During data acquisition at the Lisbon Biomechanics Laboratory, the electromyographic activity of four muscles was recorded using surface electrodes (sEMG), namely the medial and lateral heads of the gastrocnemius, soleus and tibialis anterior. This procedure is associated with concepts not clarified in this work yet, and, thus, to the scope of this section, those concepts are not described and are addressed in detail in Chapter 5. The sEMG activity will be utilized to assess the results obtained from the optimization procedure. However, during the treatment of the EMG data it was observed that the activity of the medial head of the gastrocnemius muscle was not acceptable, which might have been due to electrode motion artifact during the experimental data acquisition. Hence, the sEMG data for this muscle was disregarded.

Figure 4.23 depicts the muscle activation patterns obtained from the optimization procedure for four muscles, namely the tibialis anterior, soleus, lateral head of the gastrocnemius, and peroneus brevis. These muscles were chosen to be analyzed in detail in order to provide a comparison of the results obtained from the optimization procedure with the available experimentally acquired sEMG data and also to assess the behavior of muscles that control the two degrees-of-freedom of the ankle joint complex. Equations (4.44)-(4.46) were utilized for the optimization procedure and the obtained muscle activations are compared in Figure 4.23.

The observation of Figure 4.23 leads to the conclusion that the optimization algorithm fails to find a feasible solution that satisfies all constraints imposed to the optimization procedure for some instants of time, depending on the considered cost function. For Eqs. (4.44), (4.45) and (4.46), this unsuccessful convergence of the algorithm occurs for 17, 18 and 17 instants of time, respectively, which corresponds to, approximately, 43–60%, 43–61% and 43–60% of the gait cycle, respectively. During these instants of time, unexpected muscle activation patterns are obtained. In fact, the soleus (see Figure 4.23b) and the lateral head of the gastrocnemius (see Figure 4.23c) muscles exhibit full activation or saturation, i.e. $a^m = 1$, a result that is not consistent with the human performance during healthy gait (Neumann, 2013). This phenomenon of muscle saturation is detected regardless of the cost function utilized to determine the activations. The fact that the soleus and lateral head of the gastrocnemius are fully active or saturated may decrease the activation that the optimization algorithm attributes to other muscles, for instance, the tibialis anterior, the activation of which should be higher during gait (Neumann, 2013).

Since the sEMG data is recorded in μV and the optimization results are dimensionless, the magnitude of these two quantities cannot be compared. One approach that would allow their comparison would be to record the maximum voluntary contraction of each muscle, i.e., the maximal force-generating capacity, and normalize the sEMG data using that value. However, during experimental data acquisition, this parameter was not quantified. Although a quantitative method of comparing the results is not available, a qualitative method can be employed. Analyzing the profile of the plots in Figure 4.23, it can be concluded that, overall, the results provided by the optimization algorithm show good agreement with the sEMG data, that is, when the sEMG data indicates an increase or decrease in the muscle activity, the optimization results also follow this tendency. In terms of profile of the plots, the results obtained with the optimization procedure also agree well the scientific literature (Neumann, 2013; Rajagopal et al., 2016), except for the time steps for which no solution was found by the optimization algorithm. The results presented by Ambrósio & Silva (2005) and M. T. Silva (2003) also show full activation for some muscles. The conclusions drawn out in this paragraph are true for all three tested cost functions.

Understanding the periods of muscle activation during the gait cycle sheds light on their specific kinesiological function, which allows to more easily understand deviations from the healthy gait pattern. Observing Figure 4.23, it can be seen that the tibialis anterior muscle shows three main periods of activity. In the beginning of the gait cycle, an eccentric contraction occurs in order to decelerate the plantarflexion of the talocrural joint, which is caused by the fact that the weight of the body is applied on the most posterior part of the calcaneus. In the swing phase, from 60-80% of the gait cycle, the tibialis anterior is active and contracts concentrically in order to allow dorsiflexion of the talocrural joint and ensure safe toe clearance. From 80% to the end of the gait cycle, this muscle also contracts concentrically and contributes to preparing the foot to the heel strike of the following gait cycle. As observed in Figure 4.23, the soleus and the lateral head of the gastrocnemius muscles are active throughout most of the stance phase, with the exception of the beginning of the gait cycle. During their period of activation, these two muscles contract eccentrically in order to control the plantarflexion moment that facilitates the forward propulsion of the body. The activation magnitude of the soleus and the lateral head of the gastrocnemius muscle significantly increases during the midstance and peaks during the terminal stance phase. A rapid decrease in the activation is clear in the pre-swing phase, at around 61% of gait cycle. Due to its location relative to the ankle, the peroneus brevis controls the movements of the talocalcaneal joint. In Figure 4.23, it can be seen that this muscle is active at around 60% of the gait cycle, prior to the swing phase.

Comparing the muscle activation patterns obtained using the three tested cost functions, the results present some differences, which are more or less evident depending on the muscle under analysis (see Figure 4.23). For the tibialis anterior muscle, both the magnitude and profile plots are very similar and show no significant differences among the cost functions. The most substantial variation occurs at approximately 70-90% of gait cycle, in which the results obtained using Eq. (4.45) diverge from the other two cost functions. For the soleus and the lateral head of the gastrocnemius muscles, more significant differences can be observed. In both of these muscles, the most distinct plot is the one corresponding to Eq. (4.45). In the soleus muscle, the use of Eq. (4.45) reduces the magnitude of the muscle activation from approximately 10% to 40% of the gait cycle when compared with the other cost functions. As a result, the full activation occurs later. In turn, Eq. (4.45) increases the magnitude of the lateral head of the gastrocnemius muscle activation from approximately 10% to 40% of the gait cycle, which causes the full activation to occur earlier. No significant differences are observed for the remaining simulation time. For the peroneus brevis, the most distinct plot is the one corresponding to Eq. (4.45). The conclusions drawn out in this paragraph allow to infer that the choice of the cost function to utilize is of utmost importance and should be tailored to both the movement under analysis and the objectives to be achieved.

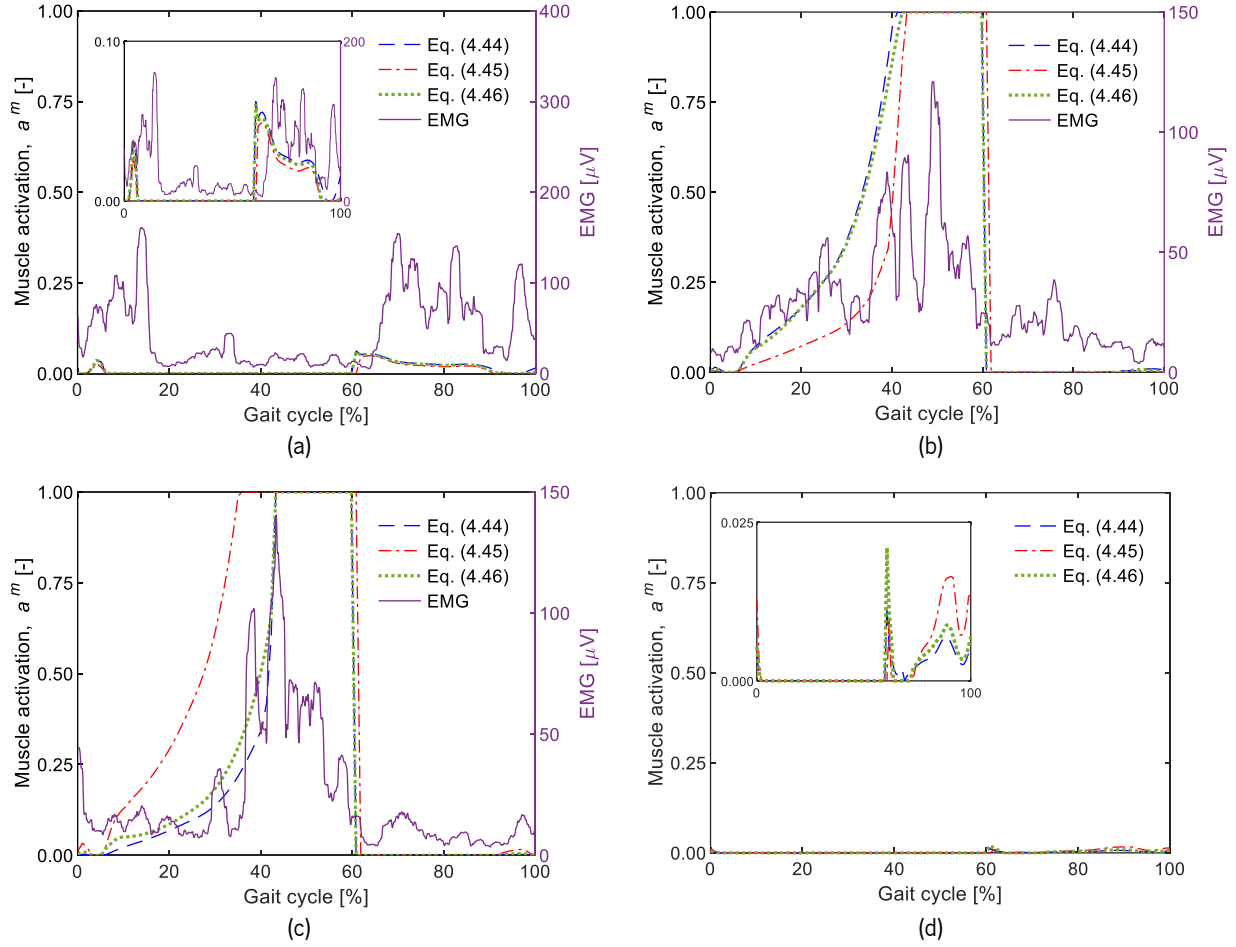


Figure 4.23 – Muscle activations, a^m , for the (a) tibialis anterior, (b) soleus, (c) lateral head of the gastrocnemius and (d) peroneus brevis muscles. The toe off occurs at 61% of the gait cycle.

In order to further investigate the justification for the optimization algorithm to converge into a solution in which some muscles are fully active during gait and other muscles demonstrate very little activation, the carpet plots for the four previously analyzed muscles are explored in detail and are displayed in Figure 4.24. Since the carpet plots are established assuming full muscle activation, that is, $a^m = 1$, they are independent of the activations generated using the different cost functions, which means that the use of either one of the three cost functions results in the same carpet plot. Figure 4.24 shows the plots using Eq. (4.46). Observing Figure 4.24, it can be concluded that all four muscles are working on the ideal force-generating zone, that is, the muscle length varies around the optimal length, l_0^m , and the muscle velocity varies around zero. In this situation, the force produced by the muscle is close to the maximum isometric muscle force, f_0^m . Hence, since the four muscles are capable of producing a magnitude of force adequate to generate the movement under analysis, i.e. gait, insufficient magnitude of force is not the cause for the optimization algorithm to produce saturated activations for some muscles. It is also important to note that all muscles perform concentric and eccentric contractions during the gait cycle, as observed from the positive and negative variations in the muscle velocity.

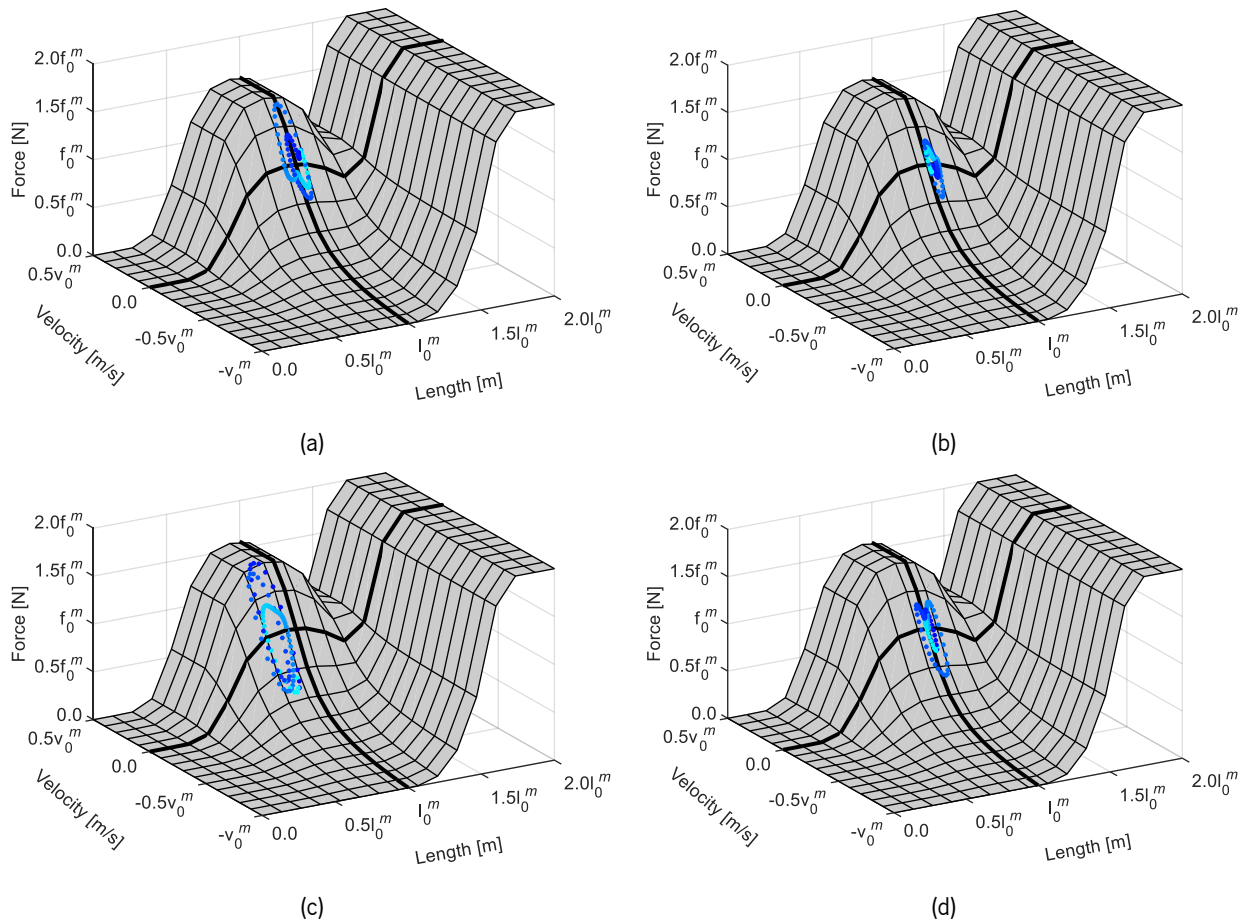


Figure 4.24 – Carpet plots for the (a) tibialis anterior, (b) soleus, (c) lateral head of the gastrocnemius and (d) peroneus brevis muscles assuming full muscle activation, that is, $a^m = 1$. The color of the plots vary from light to dark blue, which represents the beginning and end of the simulation, respectively.

Since all muscles are working on their ideal force-generating zone, the analysis of the moment arm of each muscle must be carried out in order to determine the source of optimization algorithm failure. The methodology followed in this work to calculate the moment arm of each muscle is explained in detail in Appendix E. The moment arms of the four muscles under analysis in this example of application as a function of either the talocrural or talocalcaneal joint angles are depicted in Figure 4.25. The observation of Figure 4.25 leads to the conclusion that the moment arm calculated for the tibialis anterior muscle is smaller than the results presented by Rajagopal et al. (2016), but it is within the range reported by Klein et al. (1996) for the talocrural joint. For the peroneus brevis, the obtained results are in accordance with those reported by Klein et al. (1996) for the talocrural and talocalcaneal joints. For the soleus and lateral head of the gastrocnemius, the calculated moment arms for the talocrural joint are smaller than those reported by Klein et al. (1996), Maganaris (2004), Fath et al. (2010) and Rajagopal et al. (2016). In the results obtained in Figure 4.25, the moment arms for these muscles vary between 0.63 – 1.78 cm (soleus) and 0.79 – 1.97 cm (lateral gastrocnemius) for the talocrural joint, while the literature reports higher magnitudes (approximately 4 – 6 cm). It should be noted that the results presented by Rajagopal

et al. (2016) were obtained for a 170 cm tall male subject, while the results obtained in this work refer to a 162 cm tall female subject. In addition, Klein et al. (1996) determined the muscle moment arms in embalmed foot-leg specimens, while Maganaris (2004) and Fath et al. (2010) considered *in vivo* measurements. Thus, the particular conditions under which each of those studies was conducted are different from the conditions of this study, precluding direct comparison between the results but providing a good estimate to understand the results obtained in this work.

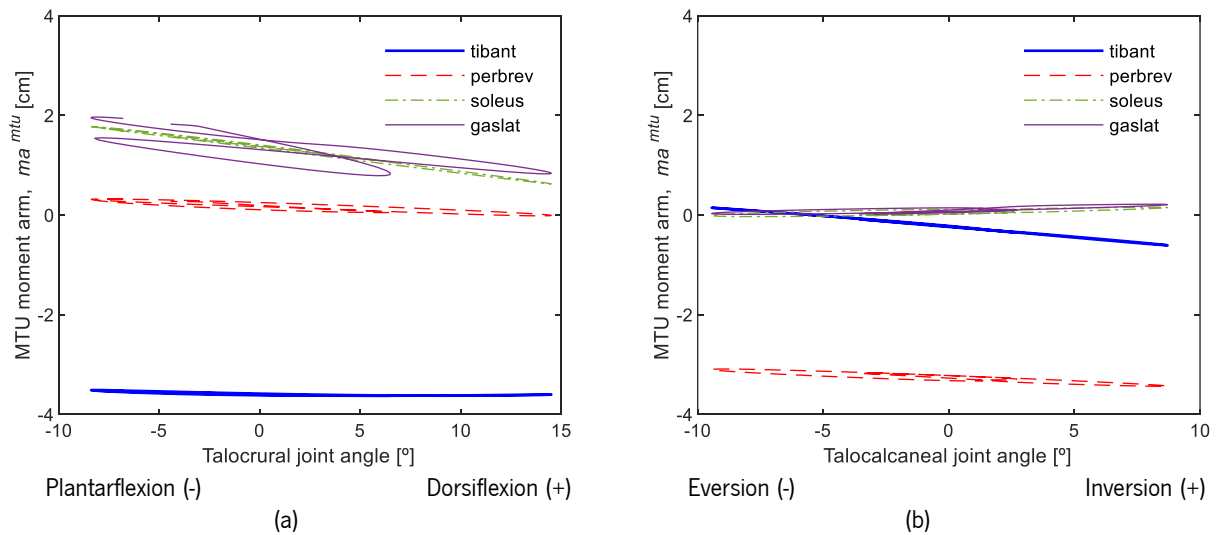


Figure 4.25 – Muscle moment arms of the tibialis anterior (tibant), peroneus brevis (perbrev), soleus (soleus) and lateral head of the gastrocnemius (gaslat) for (a) talocrural and (b) talocalcaneal joints. Positive arms indicate plantarflexion and inversion.

It is known that the soleus and the gastrocnemius (both the lateral and the medial heads) muscles together insert onto the posterior surface of the calcaneus via the Achilles tendon. Thus, they share the same insertion point (see Appendix D). The fact that the moment arm of the soleus and the lateral head of the gastrocnemius muscle is smaller than the results presented in the literature, leads to the conclusion that their insertion point may not be correctly established in the biomechanical multibody model. In order to assess whether the insertion point of these muscles is correctly placed at the posterior surface of the calcaneus, a second analysis is carried out. Since the medial head of the gastrocnemius muscle has also the same insertion point as these two muscles (see Appendix D), it must also be examined. Using the experimental data from the static trial, the location of the heel relative to the center of mass of the main foot was calculated and it was determined that the heel was placed 2 cm posteriorly relative to the defined location of the insertion point of the three muscles. In this situation, the followed approach was to relocate the insertion point of the soleus, and lateral and medial heads gastrocnemius and place it closer to the location of the heel in the anterior-posterior direction. Figure 4.26 presents a schematic representation of the procedure carried out in this work in order to relocate the insertion point of the soleus muscle. For the lateral and medial heads of the gastrocnemius muscles, the same procedure was conducted.

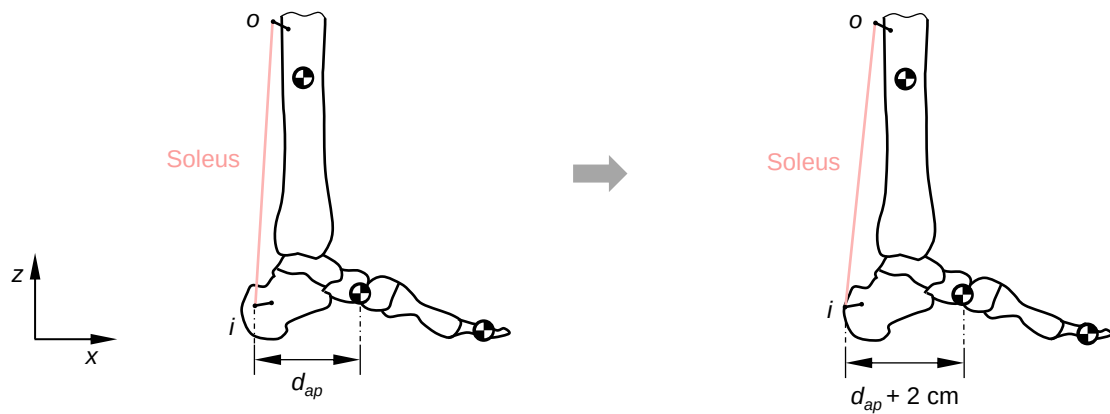


Figure 4.26 – Schematic representation of the method to relocate the insertion of the soleus in the anterior-posterior direction (x -direction). The variable d_{ap} denotes the distance from the center of mass of the main foot to the insertion point of the soleus.

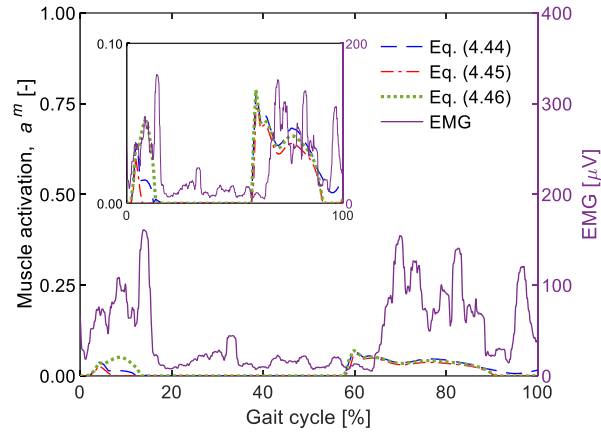
All previous analyses carried out in this section were performed in the model with the adjustment in the insertion of the soleus and gastrocnemius muscles. The obtained results are depicted Figure 4.27. Additional results can be consulted in Appendix E. The muscle activation pattern of the tibialis anterior (Figure 4.27a) did not suffer significant differences relative to the results presented in Figure 4.23a, both in magnitude and profile of the plot. The variation in the cost function utilized in the optimization procedure also did not produce substantially different activation curves. The activation of the tibialis anterior is lower than expected for gait (Neumann, 2013; Rajagopal et al., 2016). Concerning the soleus (see Figure 4.27b) and lateral head of the gastrocnemius (see Figure 4.27c), significant differences can be observed compared with Figure 4.23, as the curves using Eqs. (4.44) and (4.46) do not present full activation, which is consistent with the outcomes expected for healthy human gait (Neumann, 2013; Rajagopal et al., 2016). Although the issues of muscle saturation and optimization algorithm failure have been solved for those cost functions, the lateral gastrocnemius still presents full activation when Eq. (4.45) is utilized. On the contrary, when Eq. (4.44) is considered in the optimization procedure, the activation of the lateral head of the gastrocnemius is lower than expected for gait. In addition, the activation of the soleus using Eq. (4.45) is lower than expected for gait. Hence, Eqs. (4.44) and (4.45) do not produce physiologically consistent and reliable muscle activations. The magnitude of the activations obtained using Eq. (4.46) agree with literature (Neumann, 2013; Rajagopal et al., 2016). For the peroneus brevis (see Figure 4.27d), the results obtained with the adjusted muscle insertion indicate that the muscle activation is significantly higher when compared with Figure 4.23d from, approximately, 35-60% of the gait cycle. This section of the gait cycle was the one in which optimization failure occurred in the previous model.

Concerning the carpet plots, no significant differences are identified for the plots (e) and (h) of Figure 4.27 when compared with Figure 4.24. For plots (f) and (g), an increased range of muscle velocities is noted in comparison with Figure 4.24. The tibialis anterior (see Figure 4.27e) and lateral head of the gastrocnemius (see Figure 4.27g) exhibit high velocities during eccentric contractions, which almost leads

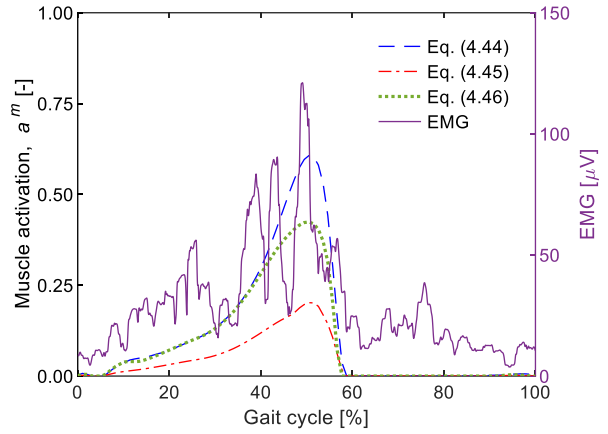
to muscle force saturation ($1.5 f_0^m$) in the force-velocity relation of Eq. (4.11), which is not expected for gait. Also, the soleus (see Figure 4.27f) and lateral head of the gastrocnemius (see Figure 4.27g) present low muscle velocities during concentric contractions, which might limit the force the muscles are capable of producing ($0.5 f_0^m$). The analysis of the carpet plots allows to conclude that all muscles contract concentrically and eccentrically during the gait cycle, and work around the ideal force-generating zone.

The moment arms of the four muscles (see Figure 4.27i and Figure 4.27j) present substantial differences when compared with Figure 4.25. The moment arms of the soleus and lateral gastrocnemius muscles vary between 2.30 – 3.55 cm and 2.48 – 3.75 cm, respectively, for the talocrural joint, which are values more consistent with literature (Klein et al., 1996; Rajagopal et al., 2016). In addition, it is important to note that the moment arms of the muscles under analysis are compatible with their function around each joint (see Table 4.4). The tibialis anterior, soleus and lateral head of the gastrocnemius are muscles responsible for the plantarflexion and dorsiflexion movements allowed by the talocrural. Hence, the moment arms of these three muscles are greater in Figure 4.27i than in Figure 4.27j. In turn, the peroneus brevis is responsible for controlling the inversion and eversion movements of the talocalcaneal joint, which explains the greater moment arm in Figure 4.27j when compared with Figure 4.27i.

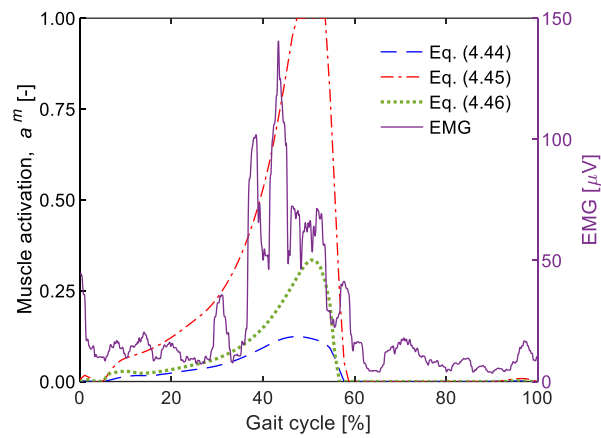
When no muscles are considered in the biomechanical multibody model, the rotational drivers of either Eqs. (3.82), (3.91) or (3.103) are responsible for controlling and guiding the corresponding degree-of-freedom and generating the movement of the joint in accordance with the prescribed experimental data. Hence, the Lagrange multiplier associated with each of those rotational drivers directly results in the moment around the joint. In turn, when considering muscles into a biomechanical model and implementing the optimization procedure described in section 4.4, the Lagrange multiplier associated with each rotational driver is no longer the moment around the joint since Eq. (4.40) is considered. Therefore, the muscles are the elements of the multibody model that are responsible for the movement of the joint, rather than the rotational driver. In this situation, the sum of the moments produced by all muscles around a joint should be equal to the total joint moment, which, in turn, should be the same as the Lagrange multiplier of the rotational driver obtained when muscles are not considered. The talocrural and talocalcaneal joint moments obtained in the present example are shown in the plots of Figure 4.27k and Figure 4.27l, respectively. The magnitude and profile of the plots agree with the literature for healthy human gait (Neumann, 2013; Rajagopal et al., 2016). However, the joint moment obtained as the sum of the moments of all muscles acting around each joint ($mom\ m$) does not coincide with the joint moment resulting from the joint driver obtained from the same model without muscles ($mom\ d$) for approximately 20-55% of gait cycle. Thus, further analyses should be performed to understand and improve the results.



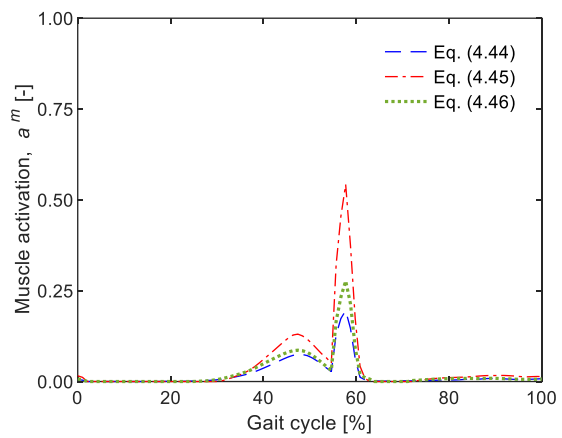
(a)



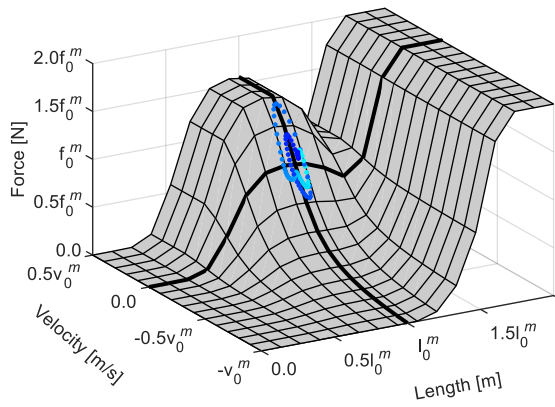
(b)



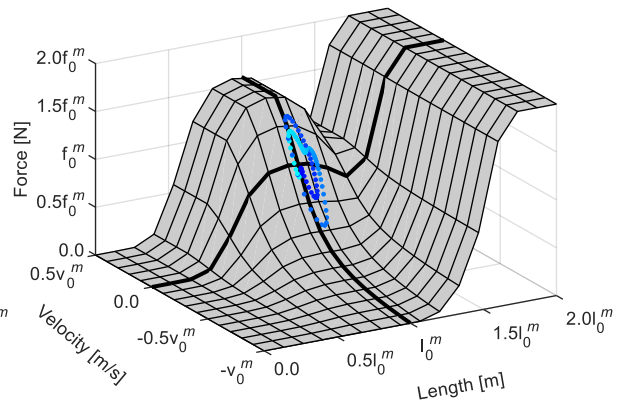
(c)



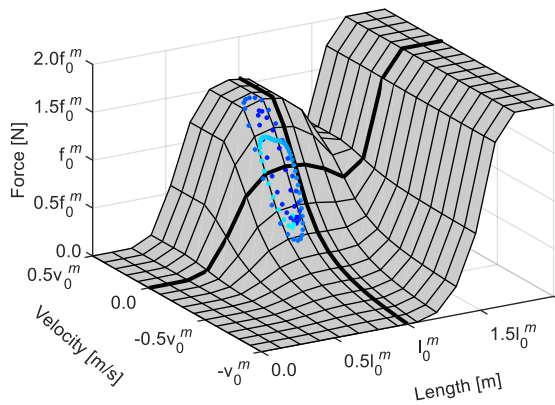
(d)



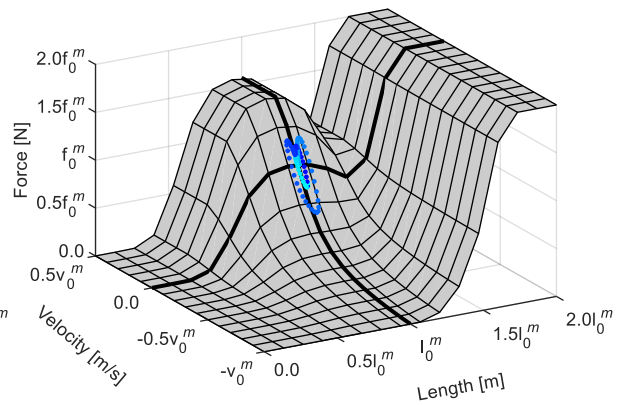
(e)



(f)



(g)



(h)

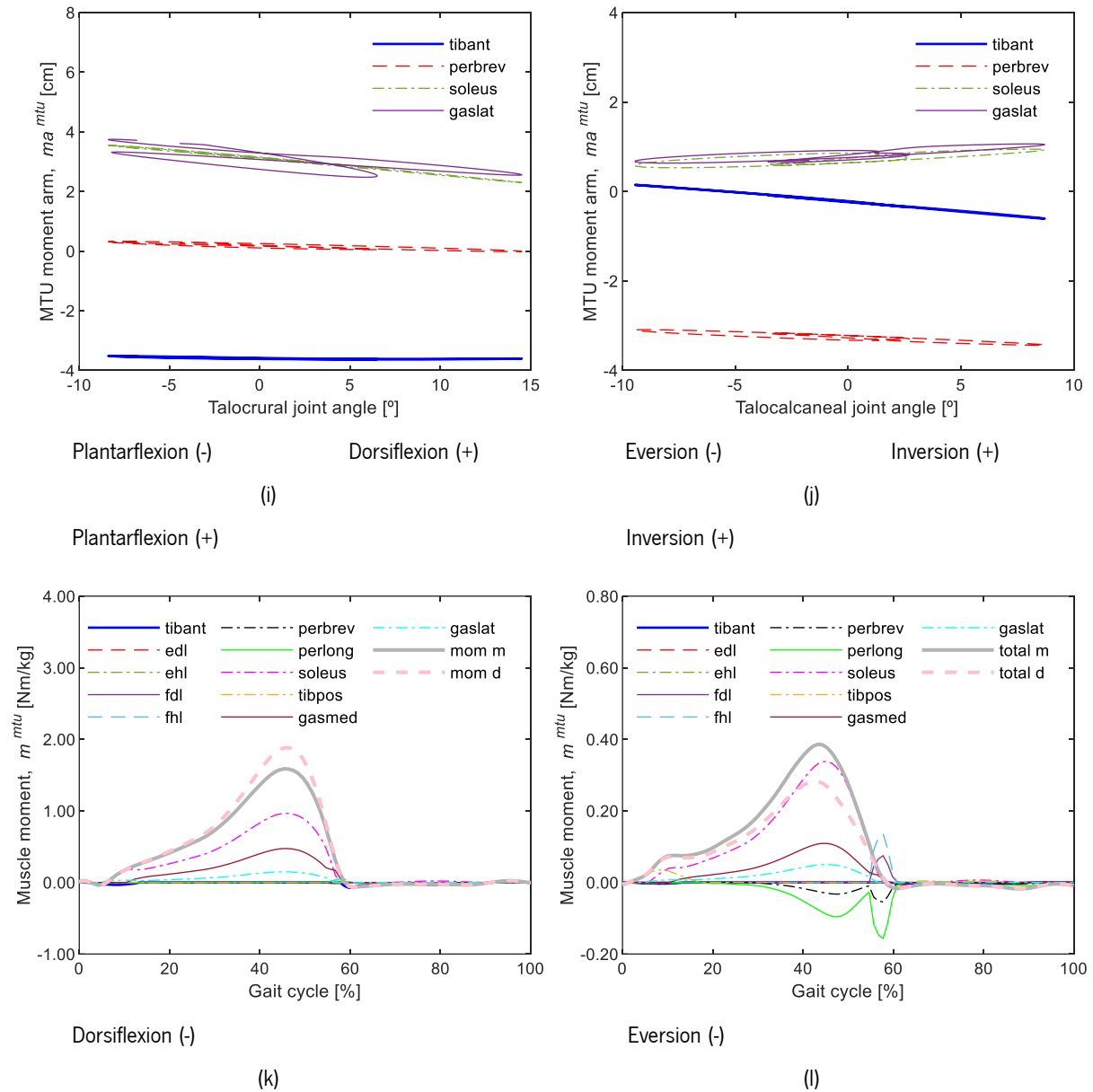


Figure 4.27 – Results for the biomechanical multibody model with the corrected insertion point. Muscle activation for the (a) tibialis anterior, (b) soleus, (c) lateral head of the gastrocnemius and (d) peroneus brevis. Carpet plots for the (e) tibialis anterior, (f) soleus, (g) lateral head of the gastrocnemius and (h) peroneus brevis. Muscle moment arms for the tibialis anterior (tibant), peroneus brevis (perbrev), soleus (soleus) and lateral head of the gastrocnemius (gaslat) for the (i) talocrural and (j) talocalcaneal joints. Positive values for the muscle moment arms indicate plantarflexion and inversion. Talocrural (k) and talocalcaneal (l) joint moments. The toe off occurs at 61% of the gait cycle.

4.6. Summary and Discussion

In the present chapter, the anatomy and physiology of the human skeletal muscles are described in detail. It is established that the functional unit that produces joint motion is the muscle-tendon unit (MTU), which consists of a muscle that has an origin and an insertion, and a tendon or an aponeurosis that interdigitates with the muscle by a musculotendinous junction. The MTU receives a signal from the

central nervous system, which stimulates the muscle fibers and causes the neurotransmitter acetylcholine (Ach) to be released into the synaptic cleft. The Ach activates the muscle fiber and provokes the release of calcium ions that participate in the muscular contraction. The force produced by the muscle is then transmitted to its adjacent tendon, which, in turn, transmits the force to the bone, resulting in joint motion.

In this work, only the muscle contraction dynamics is approached, which corresponds to the process of transforming the muscle activation into muscle force. Several mathematical models have been developed and are utilized to relate the force produced by a skeletal muscle with the resulting movement of the musculoskeletal system. The muscle model utilized here to reproduce the contraction dynamics is a variant of the Hill model and it is composed of an active contractile element arranged in parallel with an elastic element. The MTUs are spatially defined by the coordinates of a series of points connected by line segments. The first and last of these points correspond to the MTU origin ("o") and insertion ("i"), respectively, while the remaining points represent the via-points (" v_p "). In this work, the skeletal MTUs are considered as external forces acting on the system, and thus the force magnitude is assumed to be the same at any point of the MTU and equal to the total force exerted by the MTU. It is important to note that, since the number of muscle activations exceeds the number of degrees-of-freedom of the biomechanical models, a unique solution for the analytical determination of the muscle forces cannot be obtained. Thus, the solution for this problem can be found through the use of an optimization procedure, which allows to estimate the optimal muscle activations according with the minimization of cost functions that simulate the decisions taken by the central nervous system when executing a certain task.

At the end of the chapter, two examples of application are provided and discussed in detail. The first example includes a double pendulum multibody model that is utilized to validate the muscle modeling methodology considered in this work. The results allow to conclude that the implemented methodology is correctly working and producing expected results. The aim of the second example of application is to demonstrate the consideration of muscles into a more realistic biomechanical multibody model of the human lower limb. The focus of the analysis is on the ankle joint complex of the human foot. After understanding and overcoming the issue of optimization algorithm failure, the results are physiologically sound for the muscle activations, muscle moment arms and joint moments. The magnitude and profile of the plots obtained for the talocrural and talocalcaneal joint moments agree well with the literature for healthy human gait. However, the joint moment resulting from the sum of the moments of all muscles acting around each joint does not entirely coincide with the joint moment obtained from the joint driver of the same biomechanical model without muscles for approximately 20-55% of gait cycle. Thus, further analyses should be performed in order to understand and improve the results.

“The most enjoyable part of science is doing it.”

Kip Thorne, Nobel Prize in Physics 2017

5. BIOMECHANICAL MULTIBODY MODEL

In this chapter, two biomechanical multibody models are developed. The main difference between the models is associated with the detail with which the shoulder joint complex is approached. The simple model considers the glenohumeral joint only, which is formulated as a spherical joint. The detailed model includes the glenohumeral, sternoclavicular, acromioclavicular and scapulothoracic joints, which are formulated either as spherical or ellipsoidal joints. The simple model was utilized to analyze experimental gait data of the human movement acquired at the Lisbon Biomechanics Laboratory. Kinematic, kinetic and electromyographic data were recorded. The adopted acquisition protocol and the data treatment procedures are approached in detail. An important aspect to consider when acquiring experimental data of the human movement is that the processed kinematic data does not guarantee that the constraints of the biomechanical models are fulfilled. Hence, in order to correct this issue, a kinematic consistency procedure is developed and applied to the model. The chapter ends with an application example.

5.1. Description of the Multibody Model

In this work, two three-dimensional biomechanical multibody models of the human body are developed and implemented using the MATLAB in-house code MUBODYNA. Both biomechanical models share the same anthropometric parameters and the difference between them resides in the approach utilized to describe the shoulder joint complex. One model considers that the upper part of the trunk is connected to the arm via the glenohumeral joint only, while the other multibody model connects the two segments using a more detailed modeling of the shoulder joint complex, following the approach proposed by Quental et al. (2012). Currently, the biomechanical model considering a simple representation of the shoulder can be utilized for both simulation and analysis of the human movement, the last of which includes the use of experimental data, while the model with a more detailed shoulder can be utilized for simulation purposes only. The justification for this distinction is associated with the definition of the marker set protocol utilized during the experimental data acquisition procedures that are described in section

5.2. In the present work, gait is the movement chosen to be investigated in both unassisted and device-assisted analyses. The model with a detailed shoulder requires the use of a more elaborate marker set protocol in order to correctly and accurately capture the movements of all bodies and joints utilized to reproduce the actual shoulder joint complex (Quental, 2013). The increased complexity in the marker set protocol is not a feasible approach for the exclusive analysis of gait only. Considering the characteristics described in this paragraph, the first model is hereafter designated as biomechanical model with the simple shoulder or simple shoulder model, whereas the second model is referred to as biomechanical model with the detailed shoulder or detailed shoulder model.

The biomechanical model with the simple shoulder is composed of 18 rigid bodies, which are kinematically connected to each other by 17 joints. In addition to these elements, the biomechanical model with the detailed shoulder comprises four additional bodies and eight additional joints, yielding a model with 22 rigid bodies and 25 joints. Due to the adopted methodology with Cartesian coordinates discussed in section 3.1, each body of the multibody model is defined by seven coordinates, as observed in Eq. (3.1), which leads to a generalized vector of coordinates with 126 and 154 entries for the simple shoulder model and detailed shoulder model, respectively. The anthropometric parameters utilized in this work are based on Rajagopal et al. (2016) and Quental (2013), and can be consulted in Appendix F. Table 5.1 presents a complete description of the bodies and joints of both biomechanical models considered in this work to analyze the human movement.

The joints utilized to kinematically connect the rigid bodies of both models are considered to be geometrically ideal. While this is a suitable approach that is frequently utilized to simulate motor activities with large rotational and translational motions, it is deemed excessively simple when particular movement details are a concern. Nevertheless, since the objective of this work is to analyze the large motions associated with unassisted and assisted gait, the use of geometrically ideal joints is a feasible approach. The joints considered in the biomechanical multibody models include spherical, revolute, classical universal, modified universal, ellipsoidal and body-followed joints (see Table 5.1). The formulation for the spherical, revolute and classical universal joints can be consulted in P. Nikravesh (1988), while the description of the modified universal joint is detailed either in section 3.2. or in M. R. Silva et al. (2024a). The ellipsoidal joint allows five degrees-of-freedom, and it is specific for the topology of the upper limb, as described by Quental (2013). The formulation is explained in Appendix G. Finally, the body-followed joint is a type of joint specifically formulated in this work to guarantee that a body j follows the motion of a body i , thus removing the six degrees-of-freedom associated with the body j . The formulation of this joint is based on six kinematic constraints that are not explicit functions of time, and, thus, vector $\mathbf{v}$ is null.

Table 5.1 – Bodies and joints of the biomechanical models with the simple and detailed shoulder

Biomechanical model with the simple shoulder				
Body (nr.)	Joint (nr.)	Joint type	Joint DoF	Connected bodies
Lower Trunk (1) ¹	Hip (1, 5)	spherical	3	Lower Trunk – Thigh
Thigh (2, 6)	Knee (2, 6)	revolute	1	Thigh – Leg
Leg (3, 7)	Ankle joint complex (3, 7)	modified universal	2	Leg – Main Foot
Main Foot (4, 8)	Metatarsophalangeal (4, 8)	revolute	1	Main Foot – Toes
Toes (5, 9)	Back (9)	spherical	3	Lower Trunk – Upper Trunk
Upper Trunk (10) ²	Glenohumeral (10, 14)	spherical	3	Upper Trunk – Humerus
Humerus (11, 15)	Humeroulnar (11, 15)	classical universal	2	Humerus – Ulna
Ulna (12, 16)	Radioulnar (12, 16)	body-followed	0	Ulna – Radius
Radius (13, 17)	Radiocarpal (13, 17)	spherical	3	Radius – Hand
Hand (14, 18)				
Biomechanical model with the detailed shoulder				
Body (nr.)	Joint (nr.)	Joint type	Joint DoF	Connected bodies
Lower Trunk (1) ¹	Hip (1, 5)	spherical	3	Lower Trunk – Thigh
Thigh (2, 6)	Knee (2, 6)	revolute	1	Thigh – Leg
Leg (3, 7)	Ankle joint complex (3, 7)	modified universal	2	Leg – Main Foot
Main Foot (4, 8)	Metatarsophalangeal (4, 8)	revolute	1	Main Foot – Toes
Toes (5, 9)	Back (9)	spherical	3	Lower Trunk – Upper Trunk
Upper Trunk (10) ²	Sternoclavicular (10, 18)	spherical	3	Upper Trunk – Clavicle
Clavicle (11, 17)	Acromioclavicular (11, 19)	spherical	3	Clavicle – Scapula
Scapula (12, 18)	Scapulothoracic TS ³ (12, 20)	ellipsoidal	5	Scapula (TS) – Upper Trunk
Humerus (13, 19)	Scapulothoracic AI ⁴ (13, 21)	ellipsoidal	5	Scapula (AI) – Upper Trunk
Ulna (14, 20)	Glenohumeral (14, 22)	spherical	3	Upper Trunk – Humerus
Radius (15, 21)	Humeroulnar (15, 23)	classical universal	2	Humerus – Ulna
Hand (16, 22)	Radioulnar (16, 24)	body-followed	0	Ulna – Radius
	Radiocarpal (17, 25)	spherical	3	Radius – Hand

¹ The “Lower Trunk” body represents the pelvis.

² The “Upper Trunk” body includes the spine, thorax and head.

³ Scapulothoracic joint on the Trigonum Spinae Scapulae (TS) point.

⁴ Scapulothoracic joint on the Angulus Inferior (AI) point.

DoF – degree-of-freedom

The body-followed joint constrains the translational and orientational coordinates of a body j relative to the translational and orientational coordinates of a body i . Hence, six kinematic constraint equations must be formulated as

$$\Phi^{(bf,6)} = \begin{cases} \mathbf{r}_j^P - \mathbf{r}_i^P = \mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i - \mathbf{s}_i^P = \mathbf{0} \\ \mathbf{p}_j - \mathbf{p}_i = \mathbf{0} \end{cases} \quad (5.1)$$

where $\mathbf{r}_k^P$ represents the global position vector of point P located on body k , $\mathbf{r}_k$ denotes the position vector of the center of mass of body k described in global coordinates, $\mathbf{s}_k^P$ is the global position vector of point P located on body k with respect to the body's local coordinate system and $\mathbf{p}_k$ represents a vector containing three Euler parameters, e , of body k . $\Phi^{(bf,6)}$ refers to a body-followed (bf) joint constraint, containing six (6) equations. The vector $\mathbf{p}_k$ ($k = i, j$) can assume the following values

$$\mathbf{p}_k = [e_0 \quad e_1 \quad e_2] \quad (5.2)$$

$$\mathbf{p}_k = [e_0 \quad e_1 \quad e_3] \quad (5.3)$$

$$\mathbf{p}_k = [e_0 \quad e_2 \quad e_3] \quad (5.4)$$

$$\mathbf{p}_k = [e_1 \quad e_2 \quad e_3] \quad (5.5)$$

The first kinematic constraint of Eq. (5.1) establishes that the geometric center of the joint has constant coordinates with respect to any of the local coordinate systems of the connected bodies. This means that point P on body i must be coincident with point P on body j , thus restricting the relative position between the bodies. The second constraint of Eq. (5.1) ensures that the Euler parameters of body i must be the same as the Euler parameters of body j , restraining their relative orientation.

The velocity constraint equations for the proposed body-followed joint are obtained by taking the first time derivative of Eq. (5.1) yielding

$$\dot{\Phi}^{(bf,6)} = \begin{cases} \dot{\mathbf{r}}_j + \dot{\mathbf{s}}_j^P - \dot{\mathbf{r}}_i - \dot{\mathbf{s}}_i^P = \mathbf{0} \\ \dot{\mathbf{p}}_j - \dot{\mathbf{p}}_i = \mathbf{0} \end{cases} \quad (5.6)$$

Taking advantage of the condition expressed in Eq. (3.27), then Eq. (5.6) can be rearranged to be expressed in terms of the angular velocity of bodies i and j as

$$\dot{\Phi}^{(bf,6)} = \begin{cases} \dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \dot{\mathbf{r}}_i + \tilde{\mathbf{s}}_i^P \boldsymbol{\omega}_i = \mathbf{0} \\ \frac{1}{2} \left(\mathbf{G}_{j,(1:3,e+1)} \right)^T \boldsymbol{\omega}_j - \frac{1}{2} \left(\mathbf{G}_{i,(1:3,e+1)} \right)^T \boldsymbol{\omega}_i = \mathbf{0} \end{cases} \quad (5.7)$$

in which $\boldsymbol{\omega}$ is the angular velocity vector in global coordinates, e denotes the subscript associated with the Euler parameter in the entries of the vectors represented in Eqs. (5.2)-(5.5) and $\mathbf{G}$ represents the transformation matrix in terms of the Euler parameters (P. Nikravesh, 1988).

Hence, observing Eq. (5.7), the contribution of the joint to the Jacobian matrix can be defined as

$$\mathbf{D}^{(bf,6)} = \begin{bmatrix} -\mathbf{I} & \tilde{\mathbf{s}}_i^P & \mathbf{I} & -\tilde{\mathbf{s}}_j^P \\ \mathbf{0} & -\frac{1}{2} \left(\mathbf{G}_{i,(1:3,e+1)} \right)^T & \mathbf{0} & \frac{1}{2} \left(\mathbf{G}_{j,(1:3,e+1)} \right)^T \end{bmatrix} \quad (5.8)$$

The time derivative of Eq. (5.6) yields the acceleration constraint equations for this joint as

$$\ddot{\Phi}^{(bf,6)} = \begin{cases} \ddot{\mathbf{r}}_j + \ddot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i - \ddot{\mathbf{s}}_i^P = \mathbf{0} \\ \ddot{\mathbf{p}}_j - \ddot{\mathbf{p}}_i = \mathbf{0} \end{cases} \quad (5.9)$$

Since Eq. (5.9) is not expressed in terms of the angular accelerations of bodies i and j , the condition expressed in Eq. (3.31) must be utilized, yielding the following equation

$$\ddot{\Phi}^{(bf,6)} = \begin{cases} \ddot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i + \tilde{\mathbf{s}}_i^P \dot{\boldsymbol{\omega}}_i - \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i^P = \mathbf{0} \\ \left(\frac{1}{2} \boldsymbol{\omega}_j^T \dot{\mathbf{G}}_{j,(1:3,e+1)} + \frac{1}{2} (\mathbf{G}_{j,(1:3,e+1)})^T \dot{\boldsymbol{\omega}}_j \right) - \left(\frac{1}{2} \boldsymbol{\omega}_i^T \dot{\mathbf{G}}_{i,(1:3,e+1)} + \frac{1}{2} (\mathbf{G}_{i,(1:3,e+1)})^T \dot{\boldsymbol{\omega}}_i \right) = \mathbf{0} \end{cases} \quad (5.10)$$

Thus, the contribution of Eq. (5.10) to the right-hand side of the acceleration equations yields

$$\boldsymbol{\gamma}^{(bf,6)} = \begin{Bmatrix} -\tilde{\boldsymbol{\omega}}_j \dot{\mathbf{s}}_j^P + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i^P \\ -\frac{1}{2} \boldsymbol{\omega}_j^T \dot{\mathbf{G}}_{j,(1:3,e+1)} + \frac{1}{2} \boldsymbol{\omega}_i^T \dot{\mathbf{G}}_{i,(1:3,e+1)} \end{Bmatrix} \quad (5.11)$$

The body-followed joint is applied on the radioulnar joint between the radius and the ulna (see Table 5.1), forcing the radius to follow the translation and orientation of the ulna (see Figure 5.1). This procedure is carried out so that these two anatomical segments are considered as a unique body. The use of the body-followed joint precludes the movement of the radius relative to the ulna as it occurs in the human body, that is, the crossing of the radius over the ulna to allow forearm pronation or supination. Nevertheless, it facilitates experimental data acquisition and the application of the driving constraints to the model. In order to overcome this issue, a potential option would be to implement the approach proposed by Kecskeméthy & Weinberg (2005). However, in this work, the pronation and supination are guaranteed by the use of a classical universal joint at the humeroulnar articulation (see Table 5.1).

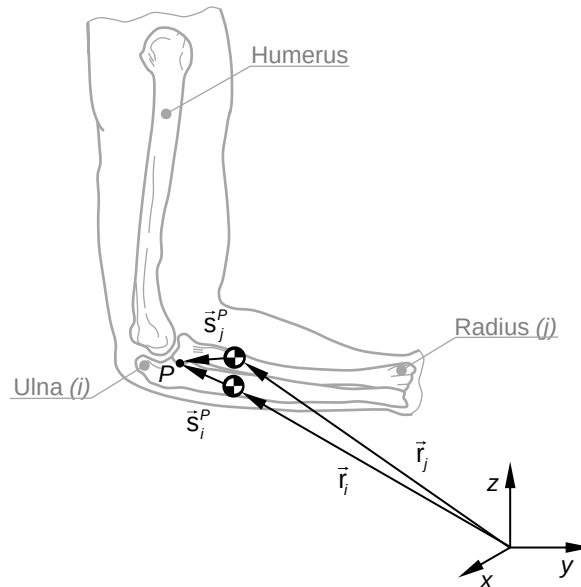


Figure 5.1 – Schematic representation of the point P used to define the body-follower joint between the ulna and radius.

Taking into consideration the bodies and joints defined in Table 5.1, the biomechanical model with the simple shoulder has 39 degrees-of-freedom, while the biomechanical model with the detailed shoulder has 47 degrees-of-freedom. Figure 5.2 illustrates the two biomechanical multibody models.

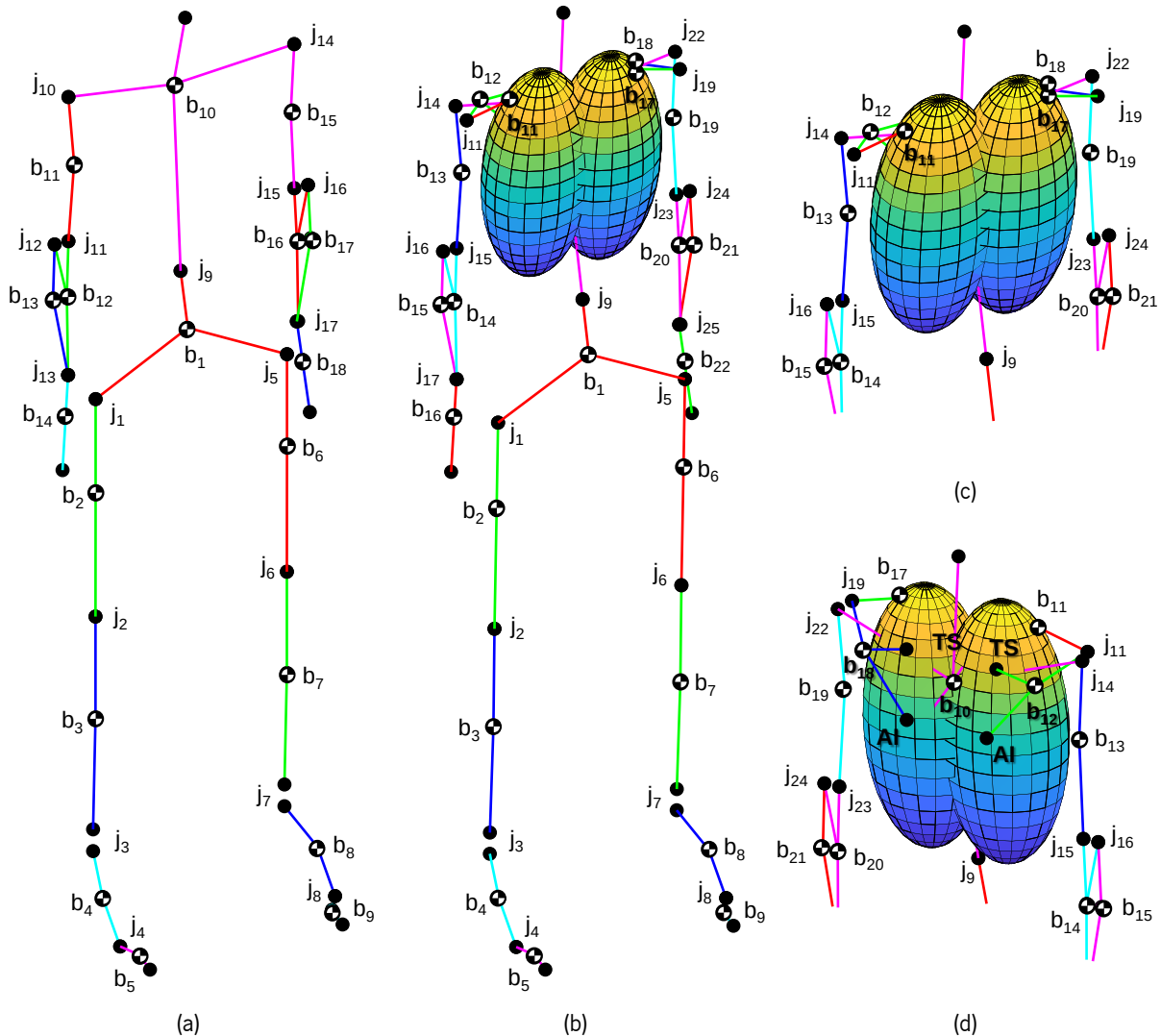


Figure 5.2 – Representation of the biomechanical multibody model with (a) the simple shoulder and (b) the detailed shoulder. Zoom of the (c) front and (d) back views of the detailed shoulder model. The letters “b” and “j” denote the body and the joint, respectively. The acronyms “TS” and “AI” represent, respectively, the Trigonum Spinae Scapulae and Angulus Inferior points of the scapulothoracic joints. The sternoclavicular joints are not shown because they are located inside the ellipsoids.

5.2. Experimental Data Acquisition

The experimental data of the human movement was acquired at the Lisbon Biomechanics Laboratory, located at the *Instituto Superior Técnico* of the University of Lisbon. Ethical approval for this study was obtained from the Ethics Commission of the *Instituto Superior Técnico* (CE-IST) in February 2024 with the reference number 3/2024 (CE-IST). In order to participate in the study, the volunteer had to be over 18 years old, be able to understand the instructions given by the laboratory technician, be able

to ambulate independently and not be in pain. Before participating in the study, a detailed explanation of the acquisition procedure was given to the volunteer. The participation was voluntary, without monetary compensation and validated by signing a term of informed consent, containing information related to the study and data acquisition. After acceptance, a form with general information (e.g. age, height, weight, gender) was filled. The anonymity was guaranteed throughout the entire study. The acquired data was post-processed using MATLAB and it can solely and exclusively be utilized for purposes arising from the study itself, such as scientific publications or communications, never revealing the volunteer's identity.

The experimental procedure does not present any risks to the volunteer, and it is a non-invasive method that involves the simultaneous use of certified systems. The Lisbon Biomechanics Laboratory (see Figure 5.3) is equipped with an optoelectronic motion capture system containing 14 Infrared ProReflex 1000 cameras (Qualisys®, Göteborg, Sweden) and one video camera (Sony HDR-HC3E). The infrared radiation emitted by the cameras meets the requirements of the EN-60825-1-2001 Class 1 and FDA CFR 1040.10 Class 1 standards, not being dangerous to the volunteer. The use of 14 cameras guarantees that all markers are visible by at least one camera during the analysis. Three force plates (AMTI OR 6-7-1000, 508 mm x 464 mm) were utilized to acquire the ground reaction forces. The video, marker trajectory, ground reaction forces and center of pressure were acquired synchronously using the Qualisys Track Manager 2.9 (Qualisys®) software. The sampling frequency was set to 100 Hz. The surface electromyography (sEMG) was acquired using the WaveX system (Cometa®) and wireless PicoX sensors.



Figure 5.3 – Lisbon Biomechanics Laboratory. Reproduced with permission from <https://lbi.tecnico.ulisboa.pt/>.

The experimental gait data of one adult female volunteer (29 years old, 162 cm, 53.340 kg) with no history of gait disorders was acquired at the Lisbon Biomechanics Laboratory. The experimental data is applied to the simple shoulder model, thus, only the bodies associated with that model are considered.

The marker set protocol with which the volunteer was instrumented in this work was developed taking into consideration the bony landmarks specified on the recommendations of the International Society of Biomechanics (Wu et al., 2002, 2005) and it is based on published studies (Fernandes et al., 2023; I. F. Roura et al., 2022). A detailed protocol for the foot was developed because this anatomical segment is divided into the main foot and toes, and due to the modified universal joint utilized to formulate the ankle (Malaquias et al., 2015; M. R. Silva, Marques, Gonçalves, et al., 2023). A schematic representation of the marker protocol is illustrated in Figure 5.4. A total of 51 passive reflective markers with a diameter of 11 mm or 19 mm were placed in palpable anatomical landmarks of the volunteer. The smaller markers were placed at the feet and hands. A cluster of four tracking markers was placed on the lateral side of each leg and arm to allow the reconstruction of problematic markers. Two markers placed on each foot, M_{48}/M_{49} and M_{50}/M_{51} , were utilized for the static acquisitions and were removed for the dynamics trials. Since M_{48}/M_{49} are placed close to other markers, namely M_{38}/M_{39} , the cameras may not be able to clearly distinguish them during the dynamic trials, potentially compromising the recorded trajectories. If M_{48}/M_{49} and M_{50}/M_{51} are needed for the dynamic trials, their trajectories can be reconstructed using the static trial.

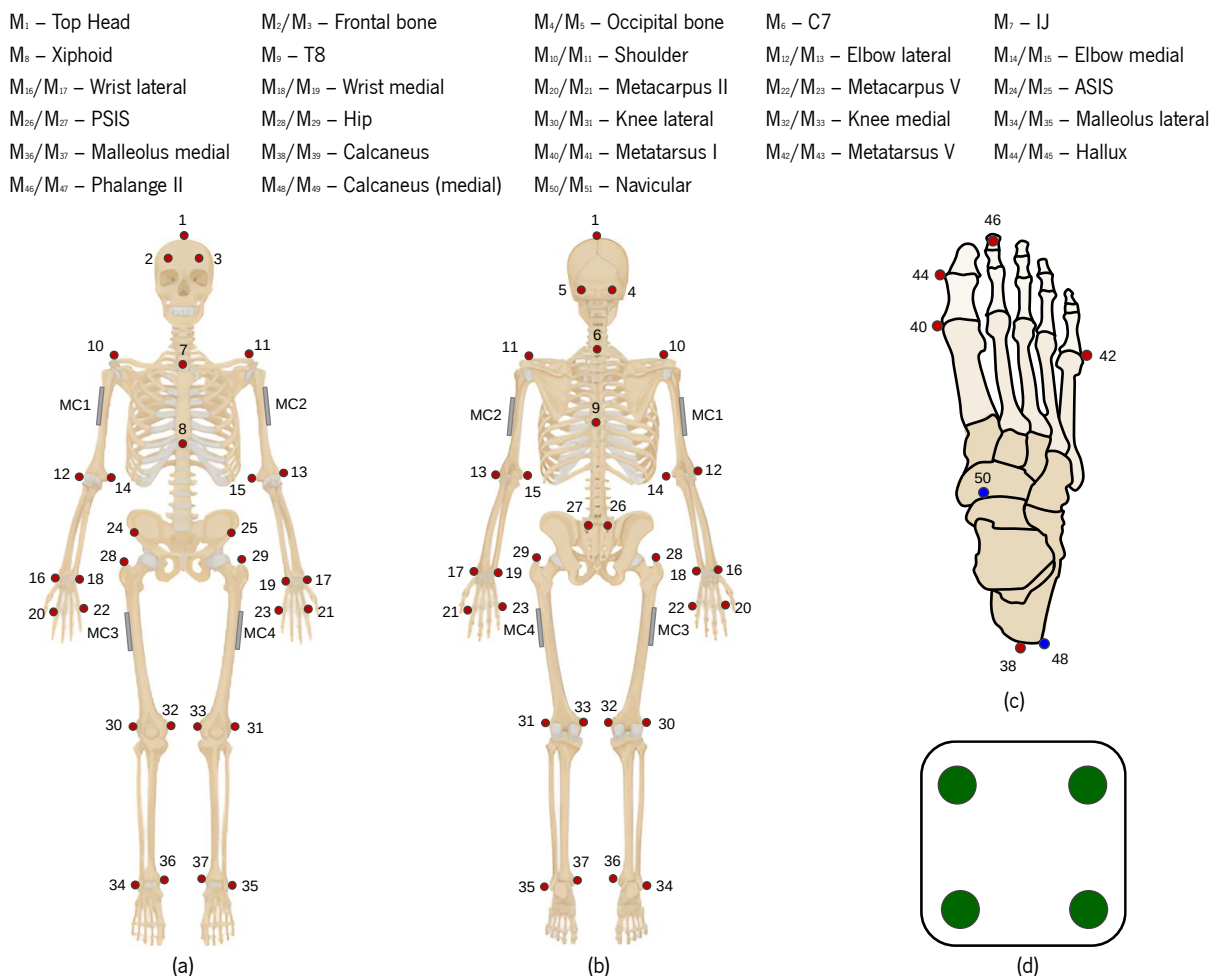


Figure 5.4 – Marker set protocol. (a) Front and (b) back views, (c) detail on the right foot and (d) marker cluster (MC). The acronyms “ASIS”, “PSIS” and “IJ” represent, respectively, the anterior and posterior superior iliac spine, and incisura jugularis.

The marker set protocol applied to the subject is displayed in Figure 5.5. There is a direct correspondence between the location of the markers and the configuration of the biomechanical model.

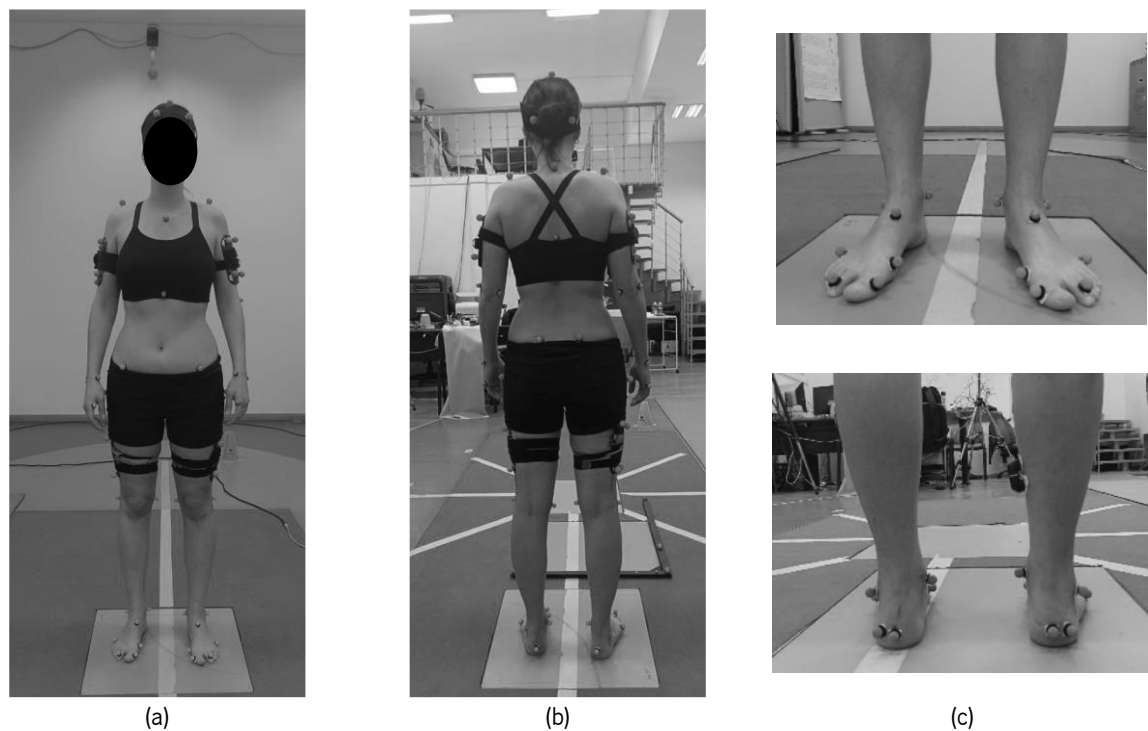


Figure 5.5 – Marker set protocol applied to the subject under analysis: (a) front and (b) back views, and (c) detail on the feet.

The sEMG activity of four muscles of the right foot, namely the tibialis anterior, soleus and medial and lateral heads of the gastrocnemius, was recorded during the dynamic trials. The placement of the wireless PicoX sensors was based on the SENIAM project (<http://www.seniam.org/>), which provides European recommendations for sensor placement for sEMG, as observed in Figure 5.6.

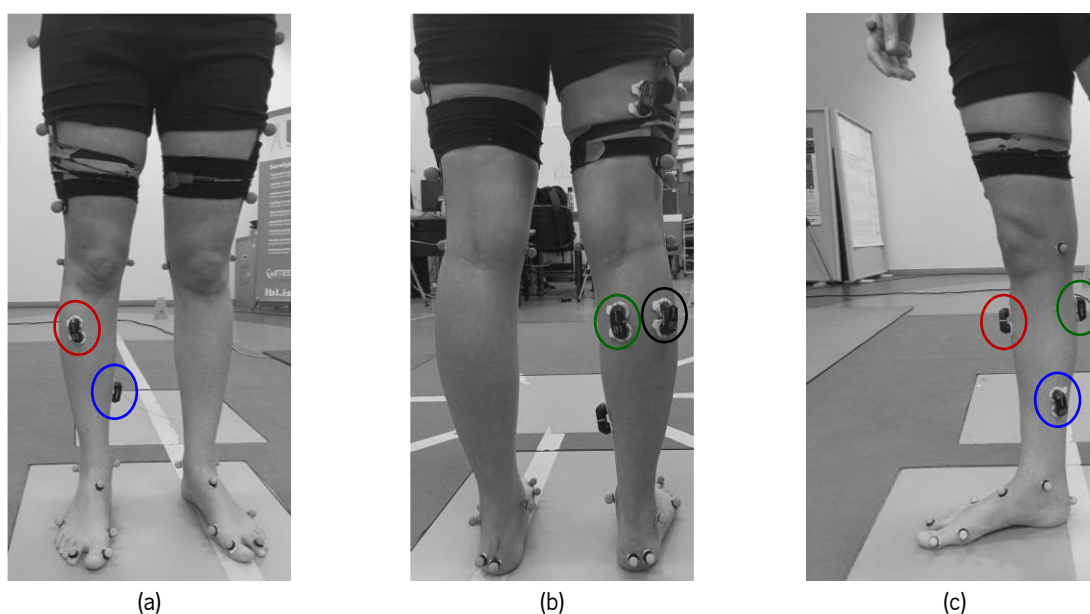


Figure 5.6 – Location of the sEMG sensors based on the SENIAM project. The red, blue, green and black circles represent the sensors placed on the tibialis anterior, soleus, gastrocnemius medial and gastrocnemius lateral, respectively.

Prior to the experimental data acquisition procedure, the subject had a period of adaptation to the experimental setup. Then, a 15-second static trial was performed in which the subject stood in the anatomical reference position. The static trial was then followed by valid dynamic trials. A trial is considered to be valid if the feet of the subject hit correctly the three force plates (one foot per plate) without adapting the cadence or step length. During the dynamic trials, the subject was asked to walk continuously with her natural cadence and no information was provided regarding the requirement of hitting the force plates. Before each dynamic trial, the subject was instructed to contract the muscles of the legs in order to indicate the beginning of the trial and facilitate the treatment of the sEMG data.

5.3. Experimental Data Treatment

As explained in section 3.1., the vector of generalized coordinates considered in this work for a given body i is expressed by seven coordinates, namely three translational coordinates of the center of mass and four Euler parameters. In addition, the vector of generalized velocities contains the linear and angular velocities of the center of mass of body i . These quantities are not directly obtained from the experimental data acquisition procedure and, thus, cannot be utilized as input to the biomechanical multibody model. Hence, the experimental gait data acquired at the Lisbon Biomechanics Laboratory must be treated and submitted to a processing procedure in order to be applied to the model.

In the present work, the duration of each analysis is defined by one complete gait cycle performed by the considered subject. A gait cycle is established as the movement beginning and ending with ground contact of the same foot, also designated as heel strike (Oatis, 2008). The cycle is divided into two phases, namely the stance and the swing, which correspond to approximately 60% and 40% of the gait cycle, respectively. During the experimental data acquisition, the subject was asked to walk back and forth over the three force plates in the x -direction in order to become familiar with the laboratory and a normal gait could be captured. Figure 5.7 illustrates a top view of the laboratory with the identification of the plates.

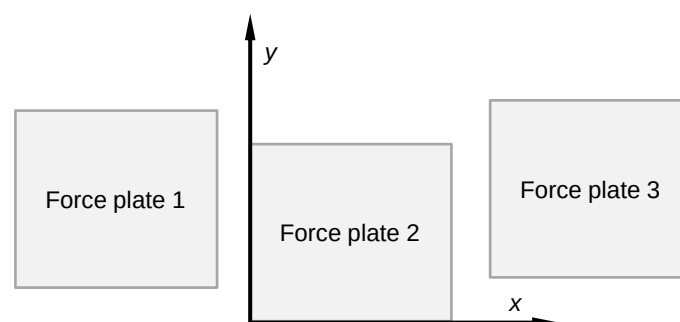


Figure 5.7 – Top view of the Lisbon Biomechanics Laboratory with the identification of the number of each force plate.

Only gait cycles in which the subject walks from the right to the left x -direction (see Figure 5.7) are considered. Hence, in the beginning of each analysis the left foot is contacting force plate 1, while the right foot is contacting the force plate 2 with the heel (heel strike). The gait cycle ends when the right foot contacts the ground in front of force plate 3 with the heel (heel strike) and the left foot is contacting force plate 3.

The treatment of the trajectory of the markers was initially done using the Qualisys Track Manager 2.9 (Qualisys®) software. An Automatic Identification of Markers (AIM) model was defined for a correct and efficient assignment of the trajectories recorded in the laboratory. The AIM model contained 67 reflective markers, which represent the 51 markers shown in Figure 5.4 and the four markers included in each of the four clusters of tracking markers. The developed AIM model is presented in Figure 5.8a, which illustrates the anatomical reference position utilized for the static trial. As explained in section 3.2, the markers M_{48}/M_{49} and M_{50}/M_{51} were utilized for calibration during the static trial and were removed for the dynamic trials. The defined AIM model with 67 markers is utilized in both the static and dynamic trials. Since markers M_{48}/M_{49} and M_{50}/M_{51} were removed in the dynamic trials, their trajectories in those trials are null. In the Qualisys Track Manager software, the acquisitions were divided by gait cycle, considering the initial contact of right foot with the force plate 2 as the first event and the initial contact of the same foot with the ground in front of the force plate 3 as the last event. Figure 5.8b and Figure 5.8c depict an example of these two events. At least 10 frames before and after the first and last events, respectively, must be considered in order to allow a correct filtering in later phases of the data treatment procedure. The treated data is exported to a *.tsv file (table-separated value) to be utilized in MATLAB.

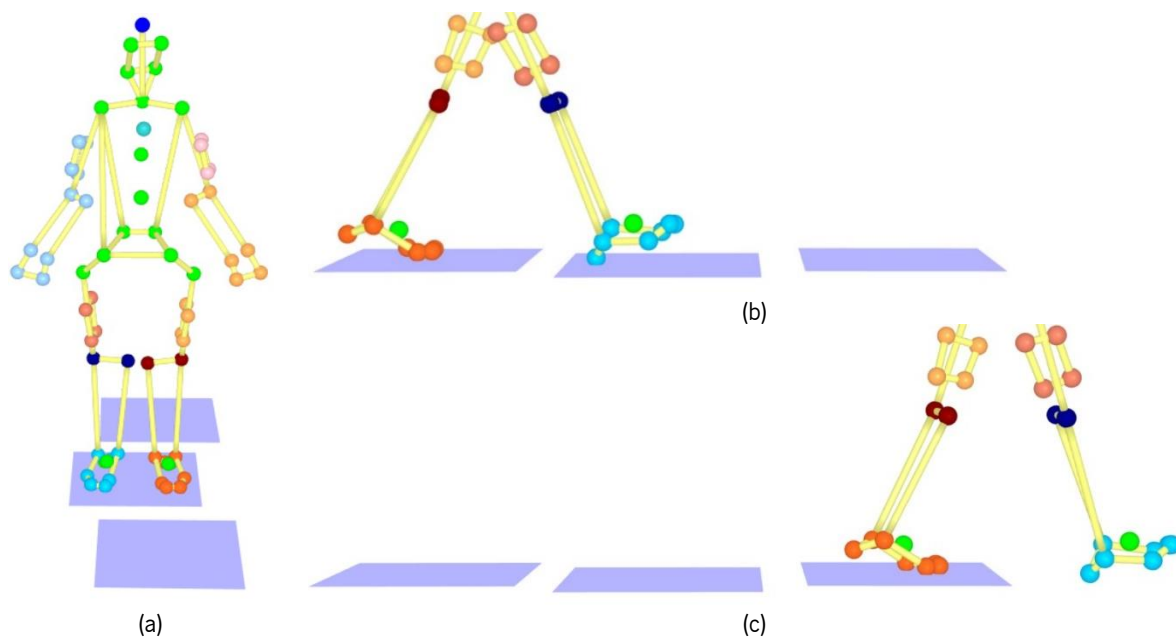


Figure 5.8 – Automatic Identification of Markers (AIM) model developed in the Qualisys Track Manager software. (a) The configuration of the model is shown for the static trial, in which the subject stood in the anatomical reference position. (b) First and (c) last events defined to delimit the gait cycle for the right foot (light blue markers).

Data filtering is often required due to several factors that introduce noise into the acquired data, such as skin motion artifact, vibration transmitted by the interaction of the foot with the ground and the occlusion of markers due to arm/leg swing. The motion capture system also introduces high-frequency low-amplitude noise. When the unfiltered data are differentiated to obtain the velocities and accelerations, the noise is amplified, resulting in errors in the dynamic analysis (Alonso et al., 2007; M. P. T. Silva & Ambrósio, 2002). When analyzing human gait, the cut-off frequency of the filter commonly ranges from 2-6 Hz, depending on the gait cadence and on the marker location. Higher cadence motion and markers placed on the upper/lower limbs require higher cutoff frequencies than slower cadence motion and markers placed on the trunk (M. T. Silva, 2003). Hence, the choice of the cutoff frequency of the filter is an important aspect to consider, since, if the selected frequency is too high, undesired noise can be transmitted to the signal, and if the frequency is too low, important features of the signal may be lost. After processing the marker data from the static and dynamic trials in the Qualisys Track Manager software, the following step was to apply a third-order low pass digital Butterworth filter with a cutoff frequency of 6 Hz. The filter attenuates the noise above the 6 Hz without affecting the frequency below the threshold, reducing the noise and smoothing the curves. When a Butterworth filter is applied to an unfiltered signal, a phase distortion occurs in the vicinity of the cut-off frequency. In order to correct the distortion, the zero-phase lag technique, which performs a second filtering of the signal in the reverse order of frames, was considered. Hence, a symmetric phase-lag that cancels the first one is introduced, eliminating the signal distortion but changing the value of the cut-off frequency. Thus, the filtered signal should be inspected to ensure correct results. Figure 5.9 provides a comparison of the data before and after the filtering process for M_{32} (see Figure 5.4) during a dynamic trial. A smoother trajectory is obtained after the filtering procedure. The filtered data of each marker was assigned to a matrix, in which each line represented the x , y and z -coordinates of the marker trajectory, and each column denoted the time step.

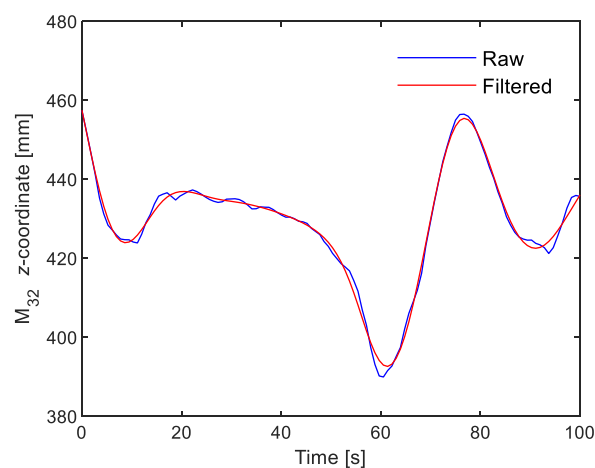


Figure 5.9 – Comparison of the z -coordinate of the M_{32} marker before (raw) and after (filtered) the filtering process.

The filtered data from the static trial was utilized to reconstruct problematic markers, including the M_{12}/M_{13} , M_{14}/M_{15} , M_{28}/M_{29} , M_{30}/M_{31} and M_{32}/M_{33} (see Figure 5.4). These markers are reconstructed because they can be significantly influenced by the motion of the skin. Besides this justification, the hip markers may also be influenced by the motion of the clothing worn by the subject during the experimental data acquisition. An example for the lateral marker of the right knee (M_{30}) is provided. The first step to reconstruct the marker is to determine the transformation matrix of the cluster plate MC3, since this is the plate associated with the anatomical segment on which the right lateral knee marker is defined (see Figure 5.4). The transformation matrix, $\mathbf{A}_{MC}$, is calculated using the following condition (see Figure 5.10)

$$\xi = \left\{ \frac{\mathbf{r}^B - \mathbf{r}^A}{\|\mathbf{r}^B - \mathbf{r}^A\|} \right\}^T \quad (5.12)$$

$$\mathbf{v}_{aux} = \left\{ \frac{\mathbf{r}^A - \mathbf{r}^C}{\|\mathbf{r}^A - \mathbf{r}^C\|} \right\}^T \quad (5.13)$$

$$\eta = \frac{\tilde{\mathbf{v}}\xi}{\|\tilde{\mathbf{v}}\xi\|} \quad (5.14)$$

$$\zeta = \frac{\tilde{\xi}\eta}{\|\tilde{\xi}\eta\|} \quad (5.15)$$

$$\mathbf{A}_{MC} = [\xi \quad \eta \quad \zeta] \quad (5.16)$$

where $\mathbf{r}^A$, $\mathbf{r}^B$ and $\mathbf{r}^C$ represent the global position vectors of markers A , B and C of the cluster plate MC3, respectively, and $\mathbf{v}_{aux}$ is an auxiliary vector.

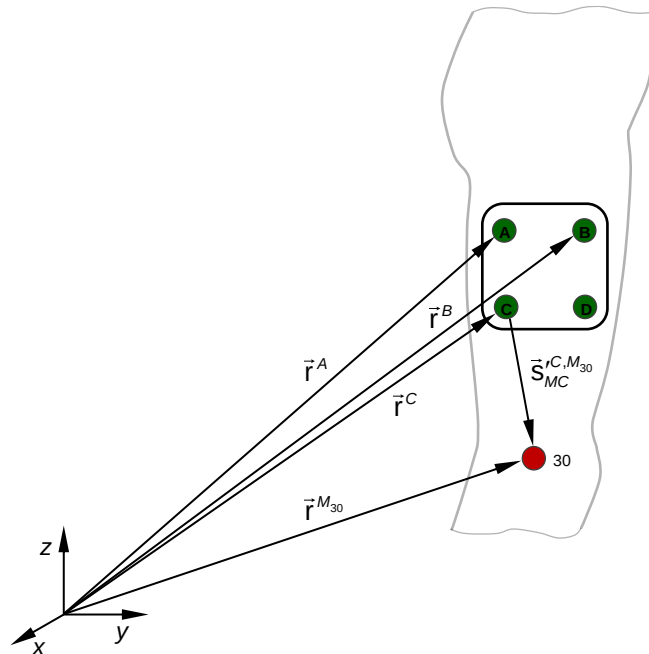


Figure 5.10 – Schematic representation of the plate containing the cluster of tracking markers with the indication of the vectors utilized to reconstruct problematic markers.

After determining the transformation matrix of the plate containing the cluster of tracking markers, the vector connecting one of the markers of the plate to the lateral marker of the right knee (M_{30}) in the local reference frame of the plate must be calculated. In this example, marker C of the plate was chosen, and the vector $\mathbf{s}_{MC}^{rC,M_{30}}$ is expressed as

$$\mathbf{s}_{MC}^{rC,M_{30}} = \mathbf{A}_{MC}^T (\mathbf{r}^{M_{30}} - \mathbf{r}^C) \quad (5.17)$$

where $\mathbf{s}_{MC}^{rC,M_{30}}$ represents the vector connecting marker C to M_{30} in local coordinates of the marker plate.

Since the vector of Eq. (5.17) is expressed in local coordinates of the plate, its magnitude and orientation are constant both in the static and dynamics trials. Hence, in the dynamic trial, the reconstructed location of the lateral marker of the right knee, $\mathbf{r}_{MC}^{M_{30},r}$, can be calculated as

$$\mathbf{r}_{MC}^{M_{30},r} = \mathbf{A}_{MC} \mathbf{s}_{MC}^{rC,M_{30}} + \mathbf{r}_{MC}^C \quad (5.18)$$

The definition of the local reference frames of each body followed the recommendations provided by the International Society of Biomechanics (Wu et al., 2002, 2005). The determination of the joint centers of the hip, $\mathbf{r}^{HJC}$, and shoulder, $\mathbf{r}^{SJC}$, were based on Davis et al. (1991) and Pàmies-Vilà (2012), respectively. The mass, and moments and products of inertia, were obtained by using the scaling factors provided in Appendix F. The length of each segment was calculated based on the data of the markers. It is important to note that the most anterior point on the toes was established using the x and y coordinates of markers M_{46}/M_{47} and the z coordinate of marker M_{44}/M_{45} , resulting in marker $M_{46.1}/M_{47.1}$. The following conditions were utilized to calculate the length of each body, l_b , of the simple shoulder model

	Right side (r)	Left side (l)
Lower Trunk ¹	$l_b = \left\ \frac{\mathbf{M}_{26} + \mathbf{M}_{27}}{2} - \frac{\mathbf{r}^{HJC,r} + \mathbf{r}^{HJC,l}}{2} \right\ $	(5.19)

Thigh	$l_b = \left\ \mathbf{r}^{HJC,r} - \frac{\mathbf{M}_{30} + \mathbf{M}_{32}}{2} \right\ $	$l_b = \left\ \mathbf{r}^{HJC,l} - \frac{\mathbf{M}_{31} + \mathbf{M}_{33}}{2} \right\ $	(5.20)
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Leg	$l_b = \left\ \frac{\mathbf{M}_{30} + \mathbf{M}_{32}}{2} - \frac{\mathbf{M}_{34} + \mathbf{M}_{36}}{2} \right\ $	$l_b = \left\ \frac{\mathbf{M}_{31} + \mathbf{M}_{33}}{2} - \frac{\mathbf{M}_{35} + \mathbf{M}_{37}}{2} \right\ $	(5.21)
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Main Foot	$l_b = \left\ \frac{\mathbf{M}_{40} + \mathbf{M}_{42}}{2} - \mathbf{M}_{38} \right\ $	$l_b = \left\ \frac{\mathbf{M}_{41} + \mathbf{M}_{43}}{2} - \mathbf{M}_{39} \right\ $	(5.22)
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Toes	$l_b = \left\ \mathbf{M}_{46.1} - \frac{\mathbf{M}_{40} + \mathbf{M}_{42}}{2} \right\ $	$l_b = \left\ \mathbf{M}_{47.1} - \frac{\mathbf{M}_{41} + \mathbf{M}_{43}}{2} \right\ $	(5.23)
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Upper Trunk ²	$l_b = \left\ \mathbf{M}_1 - \frac{\mathbf{M}_{26} + \mathbf{M}_{27}}{2} \right\ $		(5.24)
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$$\begin{array}{cc} \text{Right side (r)} & \text{Left side (l)} \\ \text{Humerus} & l_b = \left\| \mathbf{r}^{\text{SJC},r} - \frac{\mathbf{M}_{12} + \mathbf{M}_{14}}{2} \right\| \quad l_b = \left\| \mathbf{r}^{\text{SJC},l} - \frac{\mathbf{M}_{13} + \mathbf{M}_{15}}{2} \right\| \end{array} \quad (5.25)$$

$$\text{Ulna} \quad l_b = \left\| \frac{\mathbf{M}_{12} + \mathbf{M}_{14}}{2} - \frac{\mathbf{M}_{16} + \mathbf{M}_{18}}{2} \right\| \quad l_b = \left\| \frac{\mathbf{M}_{13} + \mathbf{M}_{15}}{2} - \frac{\mathbf{M}_{17} + \mathbf{M}_{19}}{2} \right\| \quad (5.26)$$

$$\text{Radius} \quad l_b = \left\| \frac{\mathbf{M}_{12} + \mathbf{M}_{14}}{2} - \frac{\mathbf{M}_{16} + \mathbf{M}_{18}}{2} \right\| \quad l_b = \left\| \frac{\mathbf{M}_{13} + \mathbf{M}_{15}}{2} - \frac{\mathbf{M}_{17} + \mathbf{M}_{19}}{2} \right\| \quad (5.27)$$

$$\text{Hand} \quad l_b = 2 \left\| \frac{\mathbf{M}_{16} + \mathbf{M}_{18}}{2} - \frac{\mathbf{M}_{20} + \mathbf{M}_{22}}{2} \right\| \quad l_b = 2 \left\| \frac{\mathbf{M}_{17} + \mathbf{M}_{19}}{2} - \frac{\mathbf{M}_{21} + \mathbf{M}_{23}}{2} \right\| \quad (5.28)$$

¹ The “Lower Trunk” body represents the pelvis.

² The “Upper Trunk” body includes the spine, thorax and head.

HJC and SJC denote, respectively, the hip and shoulder joint centers.

The total foot length was calculated as the sum of Eqs. (5.22) and (5.23), yielding values of 0.2309 and 0.2304 m for the right and left sides, respectively. Table 5.2 and Table 5.3 provide the length, mass, as well as moments and products of inertia of the bodies of the subject under analysis in the present work. The anthropometric parameters for the lower and upper parts of the trunk, as well as the mass for all bodies are presented in Table 5.2 only.

Table 5.2 – Length, mass, and moments and products of inertia for the right side of the subject under analysis

Body	l_b [m]	m_b [kg]	Moments and products of inertia [kg·m ²]					
			$I_{\xi\xi}$	$I_{\eta\eta}$	$I_{\zeta\zeta}$	$I_{\xi\eta}$	$I_{\xi\zeta}$	$I_{\eta\zeta}$
Lower Trunk ¹	0.1413	8.3758	0.0529361	0.0298152	0.0448515	0.0000000	0.0000000	0.0000000
Thigh	0.3601	6.6152	0.0741831	0.0782275	0.0194461	0.0000000	0.0000000	0.0000000
Leg	0.3661	2.6368	0.0300118	0.0304287	0.0030369	0.0000000	0.0000000	0.0000000
Main Foot	0.1702	0.8890	0.0009025	0.0026431	0.0025142	0.0000000	0.0000000	0.0000000
Toes	0.0606	0.1540	0.0000314	0.0003145	0.0000629	0.0000000	0.0000000	0.0000000
Upper Trunk ²	0.7335	19.0791	1.2303151	1.1943527	0.6303853	0.0000000	0.0000000	0.0000000
Humerus	0.2682	1.4455	0.0116486	0.0124123	0.0023758	-0.0003030	0.0004364	-0.0000485
Ulna	0.2384	0.4321	0.0022590	0.0021006	0.0003487	-0.0000115	0.0000259	0.0001844
Radius	0.2384	0.4321	0.0017285	0.0016072	0.0002668	-0.0000088	0.0000198	0.0001411
Hand	0.0785	0.3254	0.0001857	0.0001565	0.0000721	-0.0000112	0.0000242	0.0000120

¹ The “Lower Trunk” body represents the pelvis.

² The “Upper Trunk” body includes the spine, thorax and head.

Table 5.3 – Length, and moments and products of inertia for the left side of the subject under analysis

Body	l_b [m]	Moments and products of inertia [kg·m ²]					
		$I_{\xi\xi}$	$I_{\eta\eta}$	$I_{\zeta\zeta}$	$I_{\xi\eta}$	$I_{\xi\zeta}$	$I_{\eta\zeta}$
Thigh	0.3599	0.0740844	0.0781233	0.0194202	0.0000000	0.0000000	0.0000000
Leg	0.3678	0.0302917	0.0307124	0.0030652	0.0000000	0.0000000	0.0000000
Main Foot	0.1727	0.0009284	0.0027189	0.0025863	0.0000000	0.0000000	0.0000000
Toes	0.0577	0.0000285	0.0002849	0.0000570	0.0000000	0.0000000	0.0000000
Humerus	0.2608	0.0110162	0.0117384	0.0022468	-0.0002866	0.0004127	-0.0000459
Ulna	0.2430	0.0023468	0.0021822	0.0003622	0.0000120	0.0000269	0.0001916
Radius	0.2430	0.0017956	0.0016697	0.0002771	0.0000092	0.0000206	0.0001466
Hand	0.0762	0.0001751	0.0001476	0.0000680	-0.0000106	0.0000278	0.0000188

The length of the talus, which represents the length of the massless link of the modified universal joint, was calculated using the following conditions for the right and left sides, respectively

$$l_{\text{talus,r}} = \left\| \frac{\mathbf{M}_{34} + \mathbf{M}_{36}}{2} - \frac{\mathbf{M}_{48} + \mathbf{M}_{50}}{2} \right\| \quad (5.29)$$

$$l_{\text{talus,l}} = \left\| \frac{\mathbf{M}_{35} + \mathbf{M}_{37}}{2} - \frac{\mathbf{M}_{49} + \mathbf{M}_{51}}{2} \right\| \quad (5.30)$$

yielding a value of 0.0291 and 0.0280 m for Eqs. (5.29) and (5.30), respectively. The massless link vector is computed using Eqs. (5.29) and (5.30), but disregarding the norm.

The axes of rotation of each joint, $\mathbf{s}_j$, were calculated using the following conditions

	Right side (r)	Left side (l)	
Knee	$\mathbf{s}_j = \{\mathbf{M}_{32} - \mathbf{M}_{30}\}^T$	$\mathbf{s}_j = \{\mathbf{M}_{33} - \mathbf{M}_{31}\}^T$	(5.31)

Talocrural	$\mathbf{s}_j = \{\mathbf{M}_{36} - \mathbf{M}_{34}\}^T$	$\mathbf{s}_j = \{\mathbf{M}_{37} - \mathbf{M}_{35}\}^T$	(5.32)
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Talocalcaneal	$\mathbf{s}_j = \{\mathbf{M}_{50} - \mathbf{M}_{48}\}^T$	$\mathbf{s}_j = \{\mathbf{M}_{51} - \mathbf{M}_{49}\}^T$	(5.33)
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Metatarsophalangeal	$\mathbf{s}_j = \{\mathbf{M}_{40} - \mathbf{M}_{42}\}^T$	$\mathbf{s}_j = \{\mathbf{M}_{41} - \mathbf{M}_{43}\}^T$	(5.34)
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Humeroulnar	$\mathbf{s}_j = \left\{ \frac{\mathbf{M}_{12} + \mathbf{M}_{14}}{2} - \frac{\mathbf{M}_{16} + \mathbf{M}_{18}}{2} \right\}^T$	$\mathbf{s}_j = \left\{ \frac{\mathbf{M}_{13} + \mathbf{M}_{15}}{2} - \frac{\mathbf{M}_{17} + \mathbf{M}_{19}}{2} \right\}^T$	(5.35)
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Humeroulnar (Radioulnar)	$\mathbf{s}_j = \{\mathbf{M}_{14} - \mathbf{M}_{12}\}^T$	$\mathbf{s}_j = \{\mathbf{M}_{15} - \mathbf{M}_{13}\}^T$	(5.36)
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The location of each joint with respect to the local coordinate system of the connected bodies was obtained by using the scaling factors provided in Appendix F and it is presented in Table 5.4 for the subject under analysis. The location of the back joint relative to the upper and lower parts of the trunk is provided in the column associated with the right side of the body. It is important to note that the methodology proposed by Davis et al. (1991) determines the center of the hip joint relative to the local coordinate system of the pelvis (lower trunk). Hence, the values provided in Table 5.4 are those obtained from the Davis et al. (1991) methodology and not the ones calculated using the information present in Appendix F.

Table 5.4 – Location of each joint with respect to the local coordinate systems of each body for the subject under analysis

Joint	Body	Joint location (right side)			Joint location (left side)		
		ξ [m]	η [m]	ζ [m]	ξ [m]	η [m]	ζ [m]
Back	Lower Trunk ¹	-0.0255	0.0000	0.0693	-	-	-
Hip		-0.0016	-0.1104	-0.0870	0.0203	0.0852	-0.0894
Hip	Thigh	0.0000	0.0000	0.1500	0.0000	0.0000	0.1499
Knee		-0.0071	0.0024	-0.2100	-0.0071	-0.0024	-0.2099
Knee	Leg	0.0000	0.0000	0.1708	0.0000	0.0000	0.1716
Talocrural		-0.0092	0.0000	-0.1952	-0.0092	0.0000	-0.1961
Talocalcaneal ³	Main Foot	-0.0638	0.0129	0.0077	-0.0615	-0.0124	0.0074
Metatarsophalangeal ⁴		0.0761	-0.0010	-0.0309	0.0759	0.0010	-0.0308
Metatarsophalangeal ⁵	Toes	-0.0296	-0.0150	-0.0051	-0.0295	0.0149	-0.0051
Glenohumeral	Upper Trunk ²	0.0359	-0.1841	0.0558	0.0359	0.1841	0.0558
Back		0.0325	0.0000	-0.3466	-	-	-
Glenohumeral	Humerus	-0.0046	-0.0070	0.1213	-0.0045	0.0068	0.1179
Humeroulnar		-0.0046	-0.0070	-0.1470	-0.0045	0.0068	-0.1429
Humeroulnar	Ulna	-0.0023	0.0032	0.0949	-0.0024	-0.0032	0.0968
Radioulnar		-0.0023	-0.0172	0.0949	-0.0024	0.0175	0.0968
Radioulnar	Radius	-0.0023	0.0032	0.0949	-0.0024	-0.0032	0.0968
Radiocarpal		0.0022	0.0214	-0.1427	0.0022	-0.0218	-0.1454
Radiocarpal	Hand	-0.0032	0.0029	0.0329	-0.0031	-0.0028	0.0319

¹ The “Lower Trunk” body represents the pelvis.

² The “Upper Trunk” body includes the spine, thorax and head.

³ The location of the talocalcaneal joint relative to the main foot local coordinate system is scaled using the talus length.

⁴ The location of the metatarsophalangeal joint relative to the main foot local coordinate system is scaled using the distance from the talocrural joint to the metatarsophalangeal joint.

⁵ The location of the metatarsophalangeal joint relative to the toes local coordinate system is scaled with the total foot length.

In order to determine the vector of generalized coordinates, the location of the center of mass of each body of the model, as well as the corresponding Euler parameters must be calculated. The first step is to calculate the center of mass of the lower trunk, $\mathbf{r}_{lowertrunk}$, as

$$\mathbf{r}_{lowertrunk} = \frac{\left(\frac{\mathbf{M}_{24} + \mathbf{M}_{25}}{2} + \frac{\mathbf{M}_{26} + \mathbf{M}_{27}}{2} \right)}{2} \quad (5.37)$$

The lower trunk is considered to be the parent body of the biomechanical model, which means that, based on the location of the center of mass of the parent body, the location of the center of mass of the remaining bodies of the model are found using the parameters provided in Appendix F and Table 5.4. For instance, the location of the center of mass of the thigh, $\mathbf{r}_{thigh}$, is calculated using the following expression as

$$\mathbf{r}_{thigh} = \mathbf{r}_{lowertrunk} + \mathbf{s}_{lowertrunk}^{HJC} - \mathbf{s}_{thigh}^{HJC} \quad (5.38)$$

in which $\mathbf{s}_{lowertrunk}^{HJC}$ and $\mathbf{s}_{thigh}^{HJC}$ represent the global position vector of the hip joint center located on the lower trunk and thigh, respectively, with respect to their local coordinate systems.

Concerning the Euler parameters, the formulation proposed by P. Nikravesh (1988) was utilized. Based on the local reference frames of the bodies established following the recommendations provided by the International Society of Biomechanics (Wu et al., 2002, 2005), the transformation matrix, $\mathbf{A}_i$, for each body i can be found. Assuming that the nine direction cosines of $\mathbf{A}_i$ are given by

$$\mathbf{A}_i = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \quad (5.39)$$

then, the Euler parameters are obtained using the following conditions (P. Nikravesh, 1988)

$$e_0^2 = \frac{\text{tr}\mathbf{A}_i + 1}{4} \quad (5.40)$$

$$e_1 = \frac{a_{32} + a_{23}}{4e_0} \quad (5.41)$$

$$e_2 = \frac{a_{13} + a_{31}}{4e_0} \quad (5.42)$$

$$e_3 = \frac{a_{21} + a_{12}}{4e_0} \quad (5.43)$$

where $\text{tr}\mathbf{A}_i$ represents the trace of the transformation matrix $\mathbf{A}_i$, calculated as

$$\text{tr}\mathbf{A}_i = a_{11} + a_{22} + a_{33} \quad (5.44)$$

The vector of generalized velocities must also be determined. The linear velocity is computed by calculating the first time derivative of the location of the center of mass for each time step, and the angular velocity is calculated as (P. Nikravesh, 1988)

$$\boldsymbol{\omega}_i = 2\dot{\mathbf{p}}_i \mathbf{G} \quad (5.45)$$

in which $\boldsymbol{\omega}_i$ is the angular velocity vector, $\dot{\mathbf{p}}_i$ denotes the vector containing the first time derivative of the Euler parameters and $\mathbf{G}$ represents the transformation matrix in terms of the Euler parameters.

It is important to note that the above-mentioned procedures to calculate the vectors of generalized coordinates and velocities must be performed for each time step of the analysis of the experimental data.

After determining the location of the center of mass, the Euler parameters, as well as the linear and angular velocities of each body, a matrix $\mathbf{U}$ must be established as

$$\mathbf{U} = [\mathbf{r} \ \mathbf{p} \ \dot{\mathbf{r}} \ \boldsymbol{\omega}]^T \quad (5.46)$$

Matrix $\mathbf{U}$ contains 13 variables per body for each time step, resulting in 234 lines and n time steps.

Similarly to the data containing the trajectory of the markers exported from the Qualisys Track Manager software, the ground reaction forces (GRF) and center of pressure (CoP) data recorded with the three force plates for each time step were exported into a *.tsv file. Ten frames before the beginning and after the end of the gait cycle were considered, a procedure already explained for the marker trajectory data. A third order low pass digital Butterworth filter with a cutoff frequency of 20 Hz was employed. The filtered data was assigned to an 18-column matrix, where the first, second and third six columns corresponded to data associated with the first, second and third force plates, respectively. Within the six of columns of each force plate, the first three columns corresponded to the GRFs in the x , y and z directions, while the last three columns contained to the x , y and z -coordinates of the CoP. Each line of the matrix represented the time step. Since the foot of the biomechanical model is divided into two bodies, it is important to define on which body the GRFs and CoP are applied and at which time steps. In this work, it is considered that from the heel strike of the foot until the last time step on which the metatarsophalangeal joint of that foot touches the ground, the GRF and CoP data are applied to the main foot. In turn, from the first time step on which the metatarsophalangeal joint stops contacting the ground until the end of the stance phase of the gait cycle, the GRF and CoP data are applied to the toes.

The first step of the sEMG treatment was to use a 4th-order bandpass filter with 20 Hz and 200 Hz cutoff frequencies to reduce the electronic noise related to the movement and equipment, respectively. Then, the offset of the filtered signal was removed to allow its variation around zero. Finally, the data was rectified and smoothed using a root mean square window with 20 frames to the right and left sides.

5.4. Kinematic Consistency Procedure

After being subjected to the experimental data treatment procedure described in the previous section, the processed kinematic data that is utilized to reconstruct the human movement does not guarantee that the kinematic constraints associated with the biomechanical model are fulfilled. This phenomenon may occur due to the fact that the acquisition of the experimental data is done independently of the utilized model or due to the filtering procedure. The misplacement of the markers, skin motion artifact and the scaling of the anthropometric parameters can also contribute to errors that lead to non-consistent positions of the anatomical segments with respect to the kinematic structure of the multibody model (Alonso et al., 2016; Günther et al., 2003; Leardini et al., 2005; M. P. T. Silva & Ambrósio, 2002). As explained in the previous section, since the velocities of the system are obtained by polynomial interpolation of the coordinates and its time derivatives, the velocity constraint equations are also not fulfilled. Hence, violation of the constraints occurs, resulting in the determination of incorrect joint reaction forces and moments. Whenever the constraint equations and their time derivatives are satisfied, a system is said to be consistent with the kinematic data (M. P. T. Silva & Ambrósio, 2002).

In order to obtain kinematically consistent positions and velocities, a direct correction approach is employed (Marques et al., 2017; P. E. Nikravesh, 2007). Concerning the positions constraints violation, the vector of generalized coordinates of Eq. (3.1) is modified to incorporate the corrected positions as

$$\mathbf{q}^c = \mathbf{q}^u + \delta\mathbf{q} \quad (5.47)$$

where $\mathbf{q}^c$ and $\mathbf{q}^u$ represent the vectors containing the corrected and uncorrected positions, respectively, and $\delta\mathbf{q}$ denotes the set of corrections that eliminates the position constraints violation expressed as

$$\delta\mathbf{q} = -\mathbf{D}^{-1}\Phi(\mathbf{q}^u) \quad (5.48)$$

in which $\mathbf{D}$ is the Jacobian matrix and $\Phi(\mathbf{q}^u)$ represents the constraint equations associated with the uncorrected positions.

In general, the Jacobian matrix, $\mathbf{D}$, is not square, which means that $\mathbf{D}^{-1}$ does not exist. In order to overcome this issue, the Moore-Penrose inverse matrix is utilized and Eq. (5.48) can be rewritten as

$$\delta\mathbf{q} = -\mathbf{D}^T(\mathbf{D}\mathbf{D}^T)^{-1}\Phi(\mathbf{q}^u) \quad (5.49)$$

Finally, introducing Eq. (5.49) into Eq. (5.47), yields the following expression to calculate the corrected vector of the generalized coordinates at each time step

$$\mathbf{q}^c = \mathbf{q}^u - \mathbf{D}^T(\mathbf{D}\mathbf{D}^T)^{-1}\Phi(\mathbf{q}^u) \quad (5.50)$$

The kinematic constraint equations at the position level are commonly nonlinear. Therefore, Eq. (5.50) must be solved iteratively by using a numerical algorithm, such as the Newton-Raphson method (Marques et al., 2017; P. E. Nikravesh, 2007). The uncorrected positions, $\mathbf{q}^u$, are utilized as the initial guess to the method, which returns a solution after four or five iterations. Vector $\mathbf{q}^u$ is obtained from the first seven lines of Eq. (5.46).

After correcting the vector of the generalized coordinates for all time steps of the analysis, the linear and angular velocities associated with the corrected positions must be calculated. In order to obtain the new linear velocities, the corrected positions associated with the location of the center of mass of each body of the multibody model are interpolated and then the first time derivative is calculated. For the determination of the new angular velocities, Eq. (5.45) is utilized, in which the corrected Euler parameters of each body are interpolated to, then, obtain the first time derivative.

A mechanical system is said to be completely consistent with the kinematic data if the velocities and accelerations are also consistent with the underlying kinematic structure (M. P. T. Silva & Ambrósio, 2002). In this work, a forward multibody dynamics approach is adopted, in which Eq. (3.14) is solved for the vector containing the system accelerations, $\dot{\mathbf{v}}$, and the Lagrange multiplier vector, $\boldsymbol{\lambda}$. Therefore, only the kinematically consistent velocities must be determined. A similar methodology to the one presented in Eq. (5.47) is utilized to correct the vector of the generalized velocities of Eq. (3.4) as

$$\mathbf{v}^c = \mathbf{v}^u + \delta \mathbf{v} \quad (5.51)$$

where $\mathbf{v}^c$ and $\mathbf{v}^u$ denote the vectors containing the corrected and uncorrected velocities, respectively, and $\delta \mathbf{v}$ is the set of corrections that eliminates the velocity constraints violation expressed as

$$\delta \mathbf{v} = -\mathbf{D}^{-1} \dot{\Phi}(\mathbf{q}^c, \mathbf{v}^u) \quad (5.52)$$

in which $\dot{\Phi}(\mathbf{q}^c, \mathbf{v}^u)$ represents the constraint equations associated with the corrected positions and uncorrected velocities.

Considering again the concept of the Moore-Penrose inverse matrix, Eq. (5.52) results in

$$\delta \mathbf{v} = -\mathbf{D}^T (\mathbf{D} \mathbf{D}^T)^{-1} \dot{\Phi}(\mathbf{q}^c, \mathbf{v}^u) \quad (5.53)$$

Substituting Eq. (5.53) into Eq. (5.51) and considering the condition expressed in Eq. (3.7), yields the condition utilized to calculate the corrected vector of the generalized velocities at each time step

$$\mathbf{v}^c = \mathbf{v}^u - \mathbf{D}^T (\mathbf{D} \mathbf{D}^T)^{-1} (\mathbf{D} \mathbf{v} - \mathbf{v}) \quad (5.54)$$

where $\mathbf{v}$ denotes the right-hand side vector of the velocities constraint equations. It is important to recognize that vector $\mathbf{v}^u$ is obtained from the last six lines of Eq. (5.46).

5.5. Application Example: Analysis of Healthy Human Gait

In this application example, the biomechanical multibody model with the simple shoulder is utilized. The 39 degrees-of-freedom of the model are guided using the experimentally acquired data, and, thus, the developed driving constraints formulation presented in section 3.4 is considered. As previously mentioned, the pelvis is considered to be the parent body of the biomechanical model, and, therefore, the trajectory of its center of mass and its orientation are guided using Eqs. (3.67) and (3.75), respectively. The information regarding the formulation utilized to guide the remaining degrees-of-freedom of the model is provided in Table 5.5. The driving constraints utilized for the right and left sides of the model are the same.

Table 5.5 – Driving constraints utilized to guide the degrees-of-freedom of the simple shoulder model

Joint name	Joint type	Joint DoF	Movements	Driving constraint
Hip (1, 5)	spherical	3	Flexion/Extension	3.103
			Adduction/Abduction	3.103
			Internal/External Rotation	3.103
Knee (2, 6)	revolute	1	Flexion/Extension	3.82
Ankle joint complex (3, 7)	modified universal	2	Plantarflexion/Dorsiflexion	3.91
			Inversion/Eversion	3.91
Metatarsophalangeal (4, 8)	revolute	1	Flexion/Extension	3.82
Back (9)	spherical	3	Flexion/Extension	3.103
			Right/Left Lateral Flexion	3.103
			Internal/External Rotation	3.103
Glenohumeral (10, 14)	spherical	3	Flexion/Extension	3.103
			Adduction/Abduction	3.103
			Internal/External Rotation	3.103
Humeroulnar (11, 15)	classical universal	2	Flexion/Extension	3.82
			Pronation/Supination	3.82
Radioulnar (12, 16)	body-followed	0	–	–
Radiocarpal (13, 17)	spherical	3	Flexion/Extension	3.103
			Radial/Ulnar Deviation	3.103
			Pronation/Supination	3.103

DoF – degree-of-freedom

After treating the trajectory of the markers in the Qualisys Track Manager software and filtering the resulting data, the following step of the data treatment procedure was to reconstruct several problematic markers using Eqs. (5.12)-(5.18). Figure 5.11 shows the trajectory of the right hip marker, M_{28} , and the right medial elbow marker, M_{14} , in the x , y and z -directions before and after reconstruction. The trajectories of both markers in the x -direction are very similar when comparing the results before and

after the reconstruction. However, significant differences are observed in the y and z -directions. These differences demonstrate the importance of marker reconstruction, as large errors can be introduced in the calculation of the coordinates of the biomechanical model, compromising the obtained results.

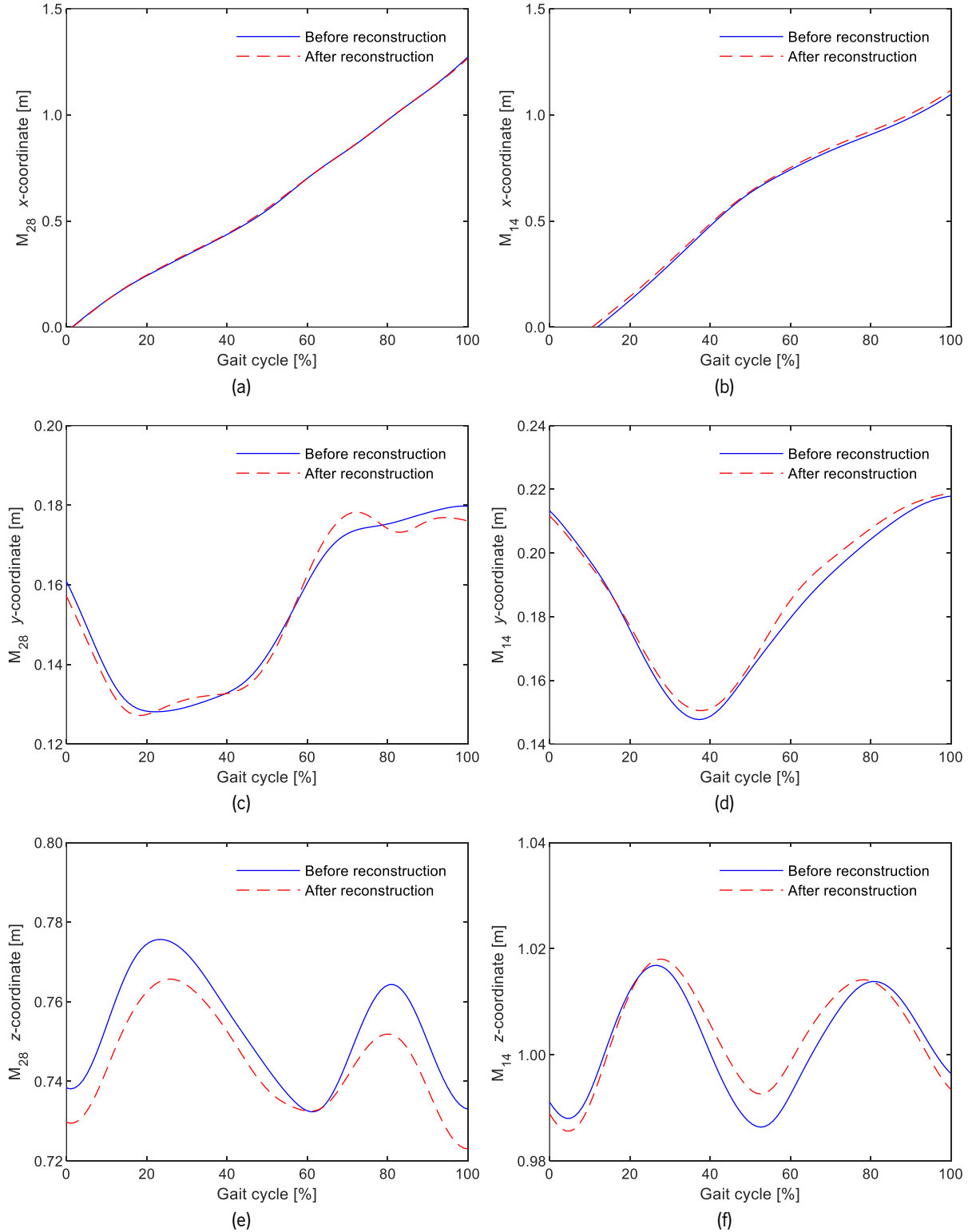


Figure 5.11 – Comparison of the trajectories of the right hip marker, M_{28} , and the right medial elbow marker, M_{14} , before and after reconstruction. Plots (a), (c) and (e) show the x , y and z -directions of the M_{28} trajectory, while plots (b), (d) and (f) show the x , y and z -directions of the M_{14} trajectory.

Besides the relevance of the marker reconstruction, it is also important to understand the impact of the kinematic consistency procedure on the quality of the obtained results. In order to investigate this issue, the biomechanical model with the simple shoulder was analyzed with and without the kinematically consistent input data. As already explained, in this work, Eq. (3.14) is solved for the vector containing the system accelerations, $\ddot{\mathbf{v}}$, and the Lagrange multipliers vector, $\boldsymbol{\lambda}$. When the non-consistent kinematic data is provided as input to the multibody model, the final time of the analysis cannot be reached. This issue was investigated, and it was concluded that high violation of the constraint equations was occurring. Hence, no solution for $\ddot{\mathbf{v}}$ and $\boldsymbol{\lambda}$ could be found through forward dynamics. In order to proceed with the analysis, inverse dynamics is utilized instead and the first branch of Eq. (3.14) is solved for $\boldsymbol{\lambda}$. The kinematically consistent accelerations are found by taking the first time derivative of the kinematically consistent velocities. Figure 5.12 shows the constraints violation before and after the kinematic consistency. It is clear that the position and velocity constraints violation disappear when the kinematically consistent data is provided as input to the biomechanical multibody model.

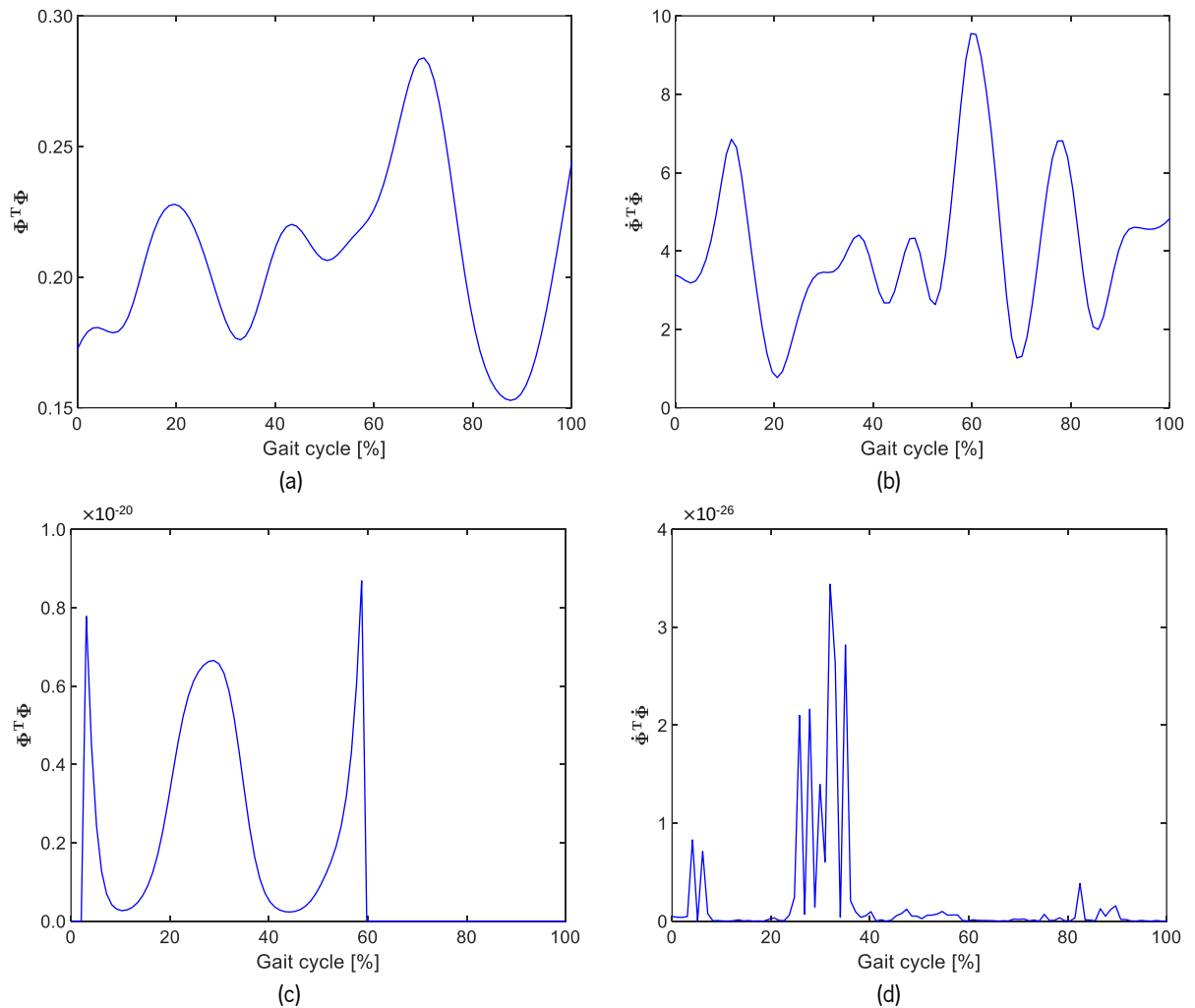


Figure 5.12 – Violation of the constraints equations at (a, c) position and (b, d) velocity levels before (a, b) and after (c, d) the application of the kinematic consistency procedure.

The observation of the configuration of the biomechanical multibody model before the application of the kinematic consistency procedure for the first time step of the analysis can also help understand, by visual inspection only, that the provided kinematic data is not consistent with the model. Figure 5.13 presents the biomechanical model with the simple shoulder before and after providing the consistent data as input. It can be concluded that, before the kinematic consistency procedure, there are constraints violations at the position level (see Figure 5.13a). This phenomenon can be confirmed from the fact that some joints are placed in a slightly different location when comparing both models, for instance, the left knee joints (j_6) and the left ankle joint complex (j_7). The application of the procedure described in section 5.4 corrects these violations, as observed in Figure 5.13b.

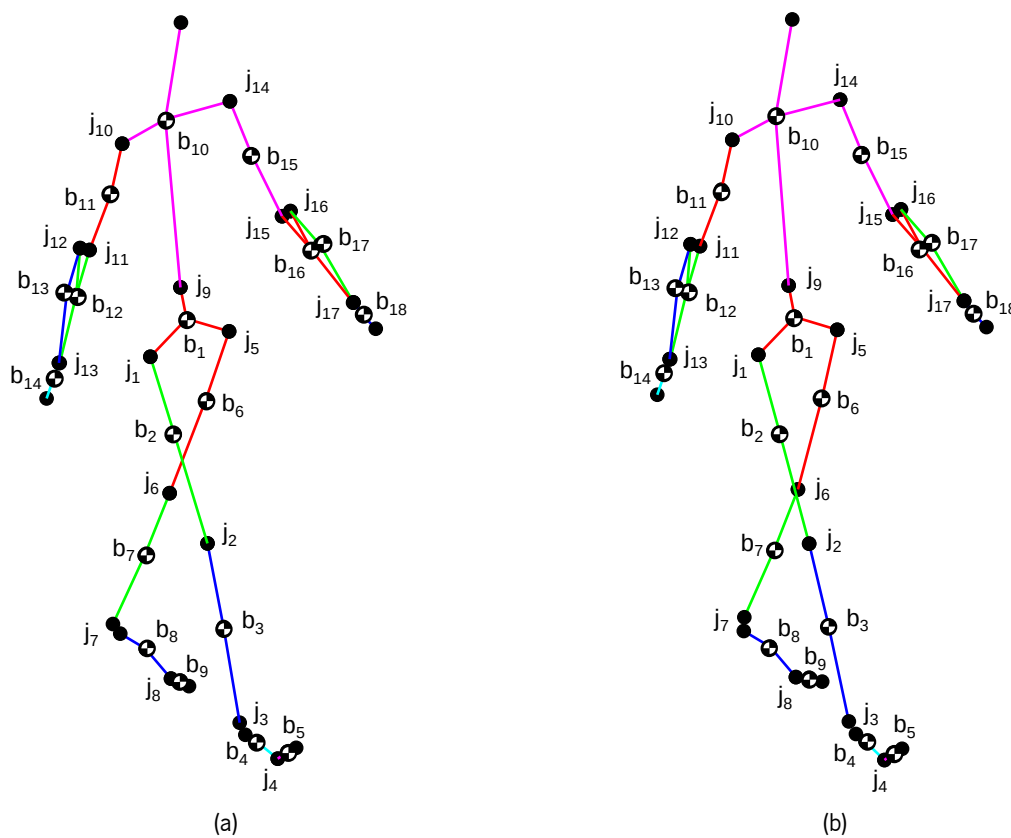


Figure 5.13 – Configuration of the biomechanical model with the simple shoulder for the first time step (a) before and (b) after the application of the kinematic consistency procedure.

The results of the joint angles and moments calculated from the inverse dynamics using the consistent and non-consistent kinematic data are also investigated and are displayed in Figure 5.14. The results were determined for all the kinematic joints composing the biomechanical model, but only those obtained for the right talocrural and talocalcaneal joints are shown. One gait cycle is considered. Significant differences are encountered when the model is provided either with the consistent or the non-consistent kinematic data. In general, when the non-consistent data is utilized, the joint angles and moments present lower and higher magnitude, respectively, than when the consistent data is considered.

In addition, it is important to note that the differences between the consistent and non-consistent curves of both joint angles and talocalcaneal joint moment are much higher than those detected for the talocrural joint moment. All the results agree well with the literature concerning the profile of the plot. However, the magnitude of the joint angles and moments obtained using the consistent data correlate better with literature (Neumann, 2013; Rajagopal et al., 2016; M. P. T. Silva & Ambrósio, 2002). This finding leads to the conclusion that the utilized kinematic consistency procedure improves the overall quality of the results provided by the biomechanical multibody model, since all kinematic constraints imposed by the structure of the model are fulfilled. In other words, the constraints violation is considered to be null. The comparison of the results obtained with the non-consistent and consistent data agrees with the results reported by M. P. T. Silva & Ambrósio (2002).

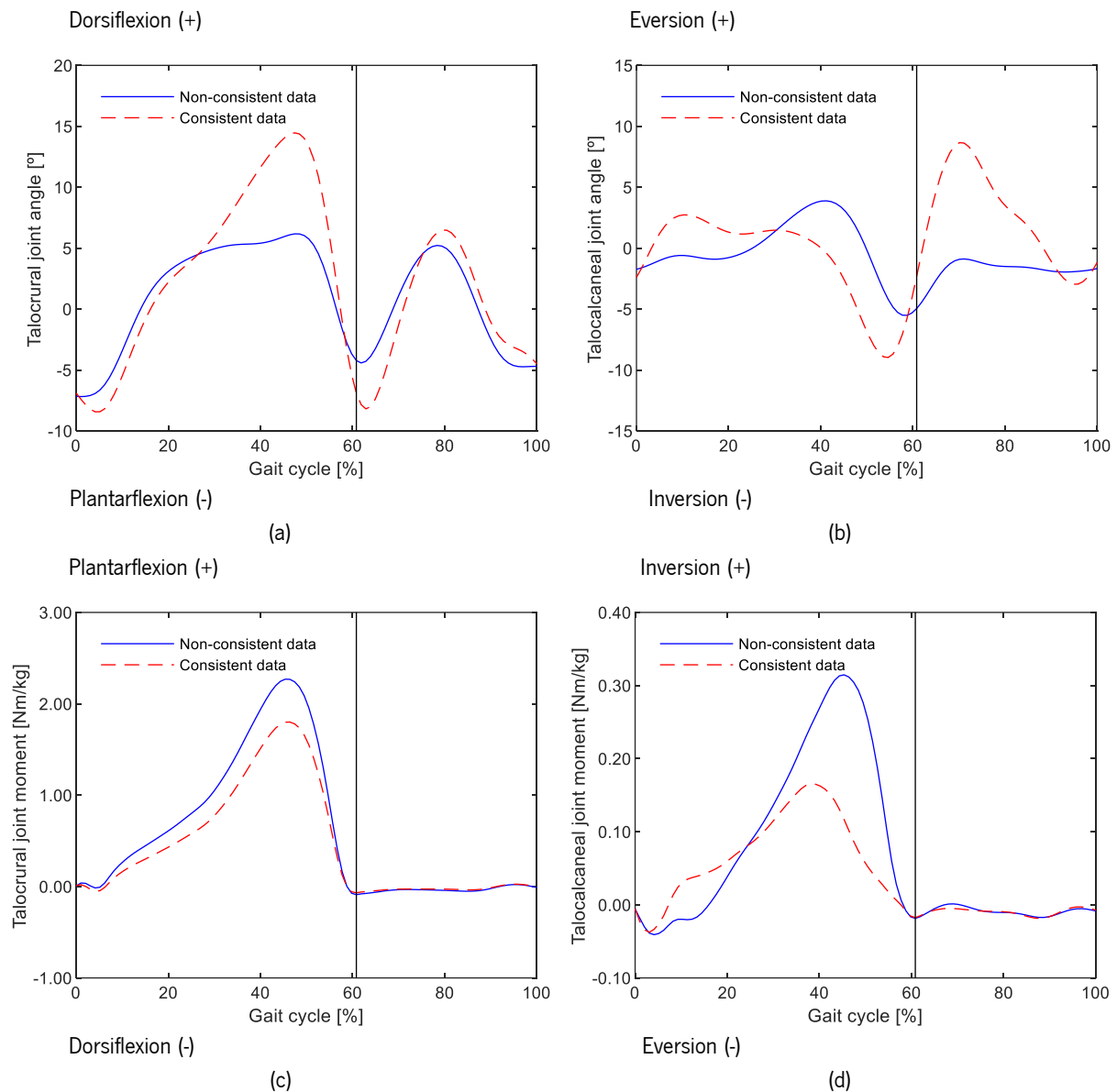


Figure 5.14 – Comparison of the angle and moment for the (a, c) talocrural and (b, d) talocalcaneal joints before and after the kinematic consistency procedure. The black vertical line indicates the toe off, which occurs at 61% of the gait cycle.

The GRF and CoP data recorded during the experimental acquisition are depicted in Figure 5.15. The results are presented after filtering and are considered for the right foot only, which is in contact with the force plate 2 (see Figure 5.7). The black solid vertical line represents the toe off, and the black vertical dashed line denotes the transition of the application of the force plate data from the main foot to the toes. Before and after the dashed line, the data is applied to the main foot and to the toes, respectively. It is important to recall that the transition from the main foot to the toes is determined by the time step at which the metatarsophalangeal joint stops contacting the ground. Observing Figure 5.15, it can be concluded that both the magnitude and profile of the plots obtained for the GRF in all directions agree with the literature (Neumann, 2013; M. T. Silva, 2003; Winter, 2009). In addition, during the gait cycle, the path of the CoP is located medially relative to the centers of mass of the main foot and toes. This result is consistent with the talocalcaneal joint angle and moment, since medial CoP provokes an eversion angle, which must be counteracted by an inversion moment (see Figure 5.14b and Figure 5.14d).

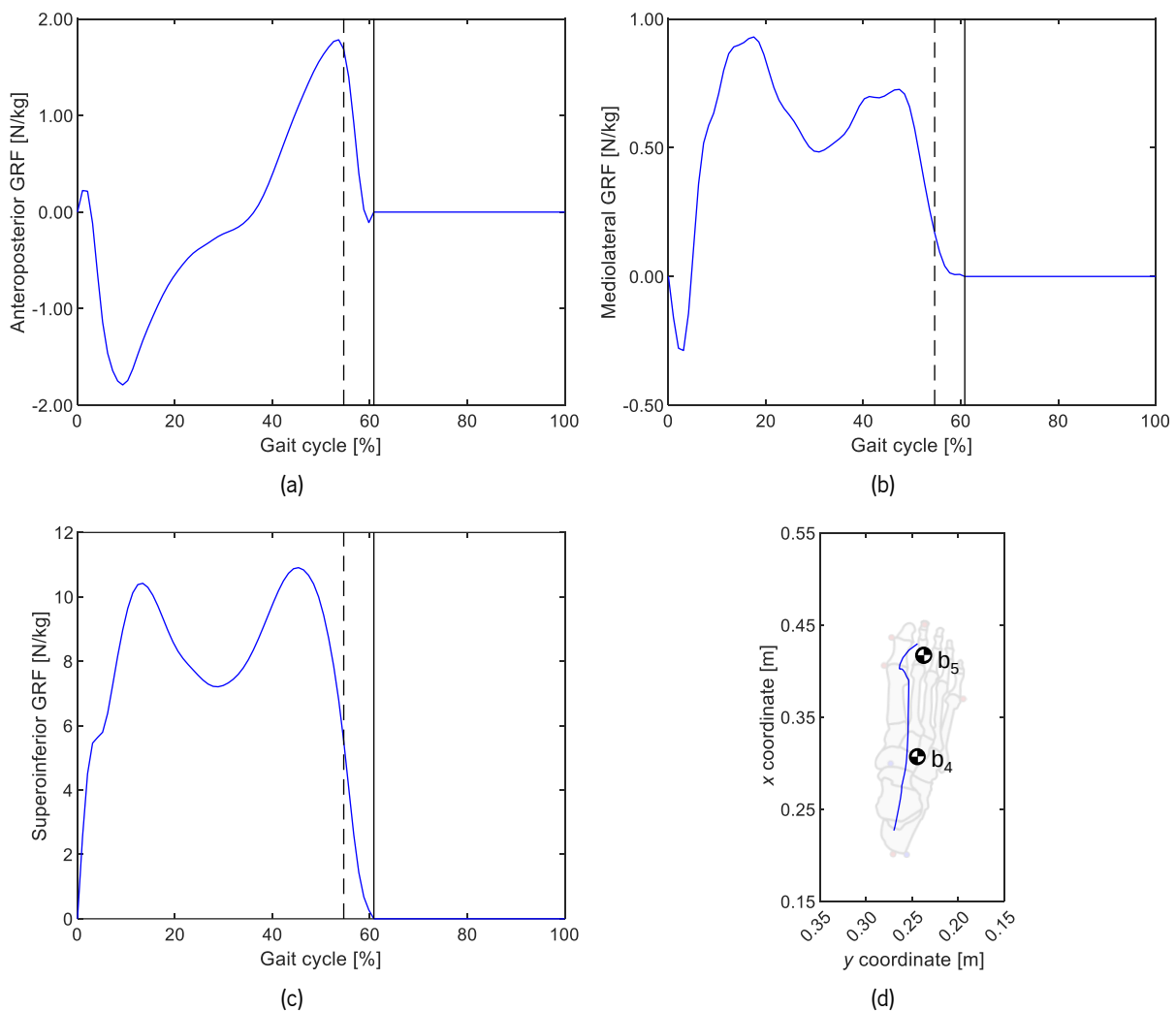


Figure 5.15 – Results obtained for the GRF in the (a) anteroposterior, (b) mediolateral and (c) superoinferior directions, and (d) path of the CoP for the right foot. The black solid vertical line indicates the toe off, which occurs at 61% of the gait cycle. The black dashed vertical line denotes the transition of the force plate data application from the main foot to the toes.

Figure 5.16 shows several snapshots of the movement of the biomechanical multibody model in the sagittal plane. The gait cycle of the right foot is shown.

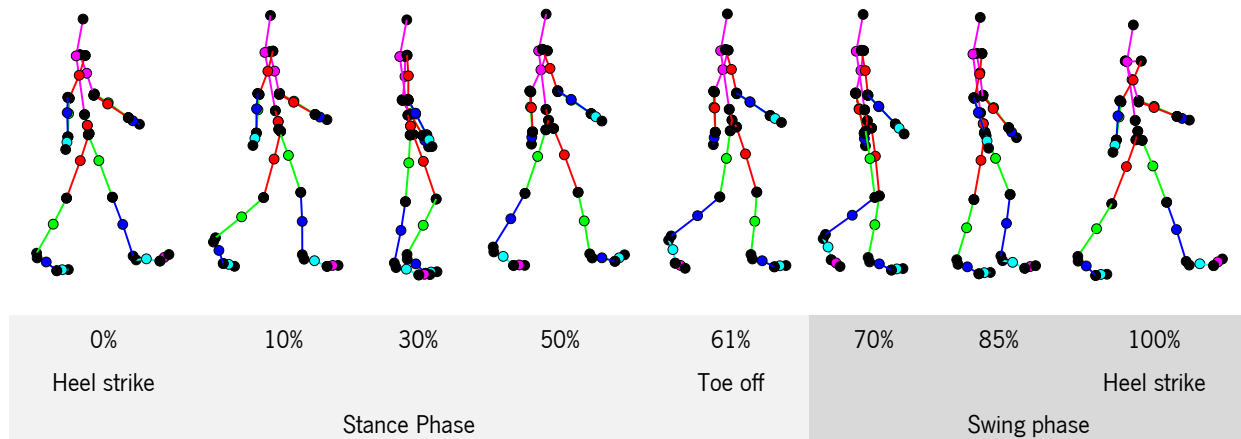


Figure 5.16 – Snapshots of the movement of the biomechanical multibody model during the gait cycle of the right foot.

5.6. Summary and Discussion

In this chapter, the complete description of the two three-dimensional biomechanical multibody models developed in this work is provided. One model considers the glenohumeral joint to connect the upper part of the trunk to the arm, and the other uses a detailed modeling of the shoulder joint complex. The detailed model includes a nontrivial ellipsoidal joint, which formulation is provided. In addition, a new type of kinematic joint has been proposed in this chapter, namely the body-follower joint, which allows to constrain the translational and orientational coordinates of a body j relative to the translational and orientational coordinates of a body i , thus removing the six degrees-of-freedom associated with body j . The formulation of the joint is presented in detail. The acquisition and treatment of the experimental data has also been a subject of analysis in this chapter, in which all the procedures carried out at the Lisbon Biomechanics Laboratory have been approached and described. Only the simple model is considered for the analysis of the data acquired at the laboratory. Following these steps, the procedure utilized to deal with the kinematic consistency of the experimental data is explained. Finally, one demonstrative example is considered in order to demonstrate the application of the data acquired at the Lisbon Biomechanics Laboratory to the biomechanical multibody model. Since the quality of the obtained results is strongly affected by the kinematic data provided as input to the model, the objective of the application example is to show the importance of the data treatment, namely the filtering and kinematic consistency procedures, as well as the process of reconstructing problematic markers. In the future, a marker set protocol for the detailed model should be developed in order to allow the analysis of movements specific to the shoulder joint complex, which is one of the most injured anatomical structures during device-assisted locomotion.

“Discovery is simply seeing what everyone else has seen - but thinking what no-one else has thought.”
Albert von Szent-Györgyi

6. DEVICE-ASSISTED GAIT

Device-assisted gait has been emerging as an important area of investigation within the multibody system dynamics methodologies. The study and analysis of this particular type of gait may help explain biomechanical demands placed on the upper limbs and establish novel design guidelines for assistive devices that improve locomotion efficiency, ultimately increasing end-user comfort. The present chapter describes the procedures carried out to study device-assisted gait. Collaborations with *Centro de Reabilitação do Norte* and ORTHOS XXI, two renowned and valuable partners, were established. The experimental protocol, methods to introduce the devices into the biomechanical model, as well as the considered approaches to handle the interactions between the device and the ground and between the device and the model are explained in detail. The chapter ends with an integrated case study.

6.1. Analysis of the Pain Perceptions Reported by Patients

Assessing the pain perceptions of patients that utilize assistive devices for their daily locomotion is of utmost importance. The knowledge acquired on this topic may be a helpful tool to understand and improve the comfort and efficiency of device-assisted locomotion. In this work, in order to understand the pain perceptions of patients using assistive devices daily, a collaboration with the *Centro de Reabilitação do Norte – Dr. Ferreira Alves*, located in Vila Nova de Gaia, Portugal, was established. The *Centro de Reabilitação do Norte* is a specialized center, that responds to the health needs of rehabilitation, targeting specifically patients with serious, complex and disabling pathologies. It is a reference center, both nationally and internationally, in the provision of differentiated healthcare, promoting the advancement of knowledge in the field of Physical Medicine and Rehabilitation, in an environment that fosters continuous training and research. Four therapeutic units exist at the *Centro de Reabilitação do Norte*, namely the Pediatric Rehabilitation Unit, the Traumatic Brain Injury Rehabilitation Unit, the Spinal Cord Injury Rehabilitation Unit, and the Stroke Rehabilitation Unit (Misericórdia do Porto, 2018). In this work, the collaboration was established with the Spinal Cord Injury Rehabilitation Unit.

Spinal cord injury (SCI) is a serious incapacitating health condition caused by damage to the anatomical structures of the spinal cord responsible for sending and receiving signals from the brain to the body and vice-versa. The condition results in disturbances to the normal sensor, motor, or autonomic functions below the injury level (Singh et al., 2014). According to the World Health Organization (WHO), SCI affects 250-500k individuals worldwide each year (World Health Organization, 2013). Despite the relatively low incidence, the consequences of SCI are disproportionally high, as it imposes a strong economic impact on the health and social systems, and strongly influences the physical, psychological and social well-being of both the patient and their family (Malekzadeh et al., 2022). In order to restore some of the mobility lost due to the SCI, patients must use assistive devices, such as crutches, walkers, wheelchairs and/or canes, which allow them to regain some degree of independence (Carver et al., 2016). However, the incorrect, repetitive and prolonged use of these devices has harmful consequences for patients, as their body weight is largely unloaded into the devices, imposing a considerable repetitive effort on the upper limbs, which are not adapted to weight-bearing tasks. This repetitive effort leads to pain, discomfort, and the development of secondary health conditions, such as carpal tunnel syndrome and shoulder/elbow tendinopathies (Manocha et al., 2021). Hence, there is an urgent need to address this issue and find strategies to prevent the onset of secondary health conditions.

In this work, the solution implemented for the first step towards achieving this goal was to develop a questionnaire to assess the pain perceptions of SCI patients during assistive device use. The questionnaire was developed under the supervision of medical doctors of the *Centro de Reabilitação do Norte*, and it is based on several validated instruments, namely the 36-item Short Form Survey (SF-36), the McGill pain questionnaire, the Quebec User Evaluation of Satisfaction with Assistive Technology (QUEST), and the standard no. 043/2011 of the Portuguese *Direção Geral da Saúde*. In order to participate in the study, the patient had to be over 18 years old, be able to read, understand and sign the informed consent, have the injury for over a year (chronic condition), be capable of independent locomotion and have clinical diagnosis of upper limb pathology. Informed consent must be signed, and the anonymity of the patients must be guaranteed. The study was approved by the Ethics Commission of *Centro Hospitalar de Vila Nova de Gaia/Espinho* in January 2024 with reference number 233/2023-1.

The developed questionnaire is presented below. Until the submission of this work, no completed questionnaires were obtained due to the fact that no patient has fulfilled the established inclusion criteria. Nevertheless, the questionnaire is ready to be utilized and promises to be a useful tool in the first step towards finding strategies to prevent secondary health conditions, that is, assessing the patients' pain perceptions. The questionnaire is not limited to SCI, and can be adapted and applied to other conditions.

1. Sociodemographic data

Gender

☐

Female

☐

Male

☐

I prefer not to say

Age

Nationality

Weight

City

Height

Professional situation

Academic Qualifications

☐

No academic qualifications

☐

High school

☐

Elementary school

☐

University

☐

Middle school

2. Questionnaire

3.1. Which assistive device do you currently use at home or in a known location?

☐

Cane

☐

Walker

☐

Crutch

☐

Walking stick

☐

Manual wheelchair

☐

Other. Specify. _____

☐

Motorized wheelchair

☐

Not applicable

3.2. Which assistive device do you currently use outside home or in an unknown location?

☐

Cane

☐

Walker

☐

Crutch

☐

Walking stick

☐

Manual wheelchair

☐

Other. Specify. _____

☐

Motorized wheelchair

☐

Not applicable

Note: If you use the assistive device in only one of the contexts (at home or outside home), please only answer the questions related to that context.

3.3. How often do you use the assistive device

at home or in a known location?

☐

Daily

☐

Other. Specify. _____

outside home or in an unknown location?

☐

Daily

☐

Other. Specify. _____

Note: If you use the same assistive device in both contexts (at home or outside home), please answer the questions related to the home context only.

3.4. Does the assistive device that you use provoke pain?

Assistive device utilized at home or in a known location

☐ Yes ☐ Sometimes ☐ No

Assistive device utilized outside home or in an unknown location

☐ Yes ☐ Sometimes ☐ No

Note: If you answered “No” to question 3.4, please proceed to question 3.5.

3.4.1. On which area or areas of your body do you feel pain?

Assistive device utilized at home or in a known location

Assistive device utilized outside home or in an unknown location

3.4.2. How do you describe the pain caused by the assistive device you use

at home? outside home?

☐☐

Acute pain
Piercing pain
Stabbing pain
Throbbing pain
Grinding

☐☐

Unpleasant sensation to touch, movement, heat, cold, pressure
Tingling/numbness
Burning/heat/burning sensation
Sensation of electric shock/sting/spike
Sensation of compression/pressure/squeezing

3.4.3. Under which circumstances do you experience pain caused by the assistive device you use

at home? outside home?

☐
☐☐
☐

I only feel pain when I use the device

The pain persists even when I am not using the device

3.4.4. How do you rate the intensity of the pain you feel?

Assistive device utilized at home or in a known location

	0		1		2		3		4		5		6		7		8		9		10
----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	----

Assistive device utilized outside home or in an unknown location

	0		1		2		3		4		5		6		7		8		9		10
----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	----

0 – No pain

4 – Light pain

8 – Severe pain

2 – Very light pain

6 – Moderate pain

10 – Very severe, unbearable pain

3.4.5. To what extent does the pain you feel prevent you from carrying out everyday activities?

Assistive device utilized at home or in a known location

	1		2		3		4		5
----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---

Assistive device utilized outside home or in an unknown location

	1		2		3		4		5
----------------------	---	----------------------	---	----------------------	---	----------------------	---	----------------------	---

1 – Totally disagree

3 – Neither agree nor disagree

5 – Completely agree

2 – Disagree

4 – Agree

3.4.6. In which of your daily activities do you feel the most pain?

Assistive device utilized at home or in a known location

Assistive device utilized outside home or in an unknown location

3.4.7. What do you currently do to relieve the pain you feel?

Assistive device utilized at home or in a known location

Assistive device utilized outside home or in an unknown location

3.4.8. In your opinion, what can be improved in the assistive device you use to relieve your pain?

Assistive device utilized at home or in a known location

Assistive device utilized outside home or in an unknown location

3.5. Are there any observations or comments you would like to make about this study?

3. Clinical data (to be filled in by the medical doctor)

Neurological level of injury		Date of injury	
AIS* classification		Etiology of injury	
AIS* sensory level		Neuromotor condition	
AIS* motor level		Other conditions	
Syndrome (if applicable)			

* AIS – American Spinal Injury Association Impairment Scale (Roberts et al., 2017)

6.2. Characterization of the Considered Assistive Device

After analyzing the scientific literature presented in Chapter 2, it was concluded that the research and interest in studying crutch-assisted locomotion has been rising over the last years. It is, therefore, the focus of the remaining sections of this chapter to investigate this type of assistive device.

In order to study and analyze crutch-assisted gait, in this work, the first step was to establish a collaboration with ORTHOS XXI, which is a European manufacturer of a wide of range of orthopedic and hospital equipment located in Guimarães, Portugal. Over the course of more than 30 years, ORTHOS XXI has grown and consolidated, becoming a recognized and respected company and a reference in the area of medical equipment. The company is driven by the conviction that their products contribute daily to improving the quality of life and satisfying the needs of their customers. The majority of the products developed and commercialized by the company are classified as class I medical devices and bear the CE mark, in accordance with the Regulation (EU) 2017/745, and are registered in the competent Authority *Infarmed*. The products are tested by accredited and independent entities, namely the *Instituto de Biomecánica de Valencia*, in Spain. The company is also certified according to the EN ISO 9001 standard (Orthos XXI - European Inclusive Solutions, 2024).

Two C8 closed cuff forearm crutches were provided by ORTHOS XXI, as it can be observed in Figure 6.1. The company recommended the use of this crutch model due to the fact that it is the most frequently requested model by their customers. The C8 closed cuff crutch has an articulated cuff and allows for double adjustment in height, which means that the adjustments can either be achieved below or above the handle. The double adjustment allows for more height options for taller users.



Figure 6.1 – The C8 closed cuff crutch provided by ORTHOS XXI (Orthos XXI - European Inclusive Solutions, 2024).

In this work, a three-dimensional computer-aided design (CAD) model of the C8 crutch was developed in Solid Edge. Only one CAD model was constructed because, according to ORTHOS XXI, there is no difference between the crutches, as they can be utilized either on the left or right sides of the user. Figure 6.2 depicts the CAD model of the crutch developed in this work.



Figure 6.2 – The CAD models of the (a) C8 closed cuff crutch and (b) mechanical components. The figure is not to scale.

Table 6.1 presents the materials of the mechanical components presented in Figure 6.2. A distinction is made between the materials utilized at ORTHOS XXI to produce the crutch and the materials considered in Solid Edge. This distinction must be made since the materials in Solid Edge do not exactly match the ones utilized by the company. In order to minimize the error and select materials in Solid Edge with the closest possible mechanical properties to those utilized at ORTHOS XXI, the technical datasheets of each material were consulted, and a reasonable approximation was accomplished. Inaccurate selection of the materials in Solid Edge may lead to errors in the estimation of the crutch center of mass and inertia.

Table 6.1 – Materials of the mechanical components constituent of the C8 closed cuff crutch produced at ORTHOS XXI

Mechanical Component	Material utilized at ORTHOS XXI	Material considered in Solid Edge
Cuff	Polyamide 6 (PA6)	Nylon
Tubes	Anodized aluminum	Aluminum, 3004
Tube inserts	Thermoplastic elastomer with polypropylene	Polyvinyl chloride (PVC)
Handle	Polyamide 6 (PA6)	Nylon
Stopper	Polyoxymethylene Acetal copolymer	Polyvinyl chloride (PVC)
Tip	Thermoplastic elastomer	Polyvinyl chloride (PVC)

6.3. Experimental Data Acquisition and Treatment

Similarly to the unassisted gait analysis, the experimental data of crutch-assisted gait was acquired at the Lisbon Biomechanics Laboratory and ethical approval for the study was obtained from the Ethics Commission of the Instituto Superior Técnico (CE-IST) in February 2024 with the reference number 3/2024 (CE-IST). The eligibility criteria, as well as all the procedures explained to the volunteer before participating in the study are the same as the ones described in section 5.2 for unassisted gait. The anonymity of the volunteer was guaranteed throughout the entire duration of the study.

One adult female volunteer (29 years old, 162 cm, 53.340 kg) with no history of gait disorders was considered. The acquired experimental data is utilized on the simple shoulder model. Hence, the marker set protocol applied on the volunteer is the one described in section 5.2 and it is depicted in Figure 5.4 and Figure 5.5. Concerning the marker set protocol for the crutch, a total of 12 passive reflective markers with a diameter of 11 mm or 19 mm were placed along the crutch surface. Two markers were located on each side of the crutch cuff, M_1 and M_2 , and handle, M_3 and M_4 . Two additional markers were placed at the front and back of the crutch handle, M_5 and M_6 . Markers M_7 and M_8 were placed on the lateral side of the middle and inferior tubes, and four markers were added at the crutch tip, M_9 , M_{10} , M_{11} and M_{12} . The marker set protocol developed for the crutches is displayed in Figure 6.3.

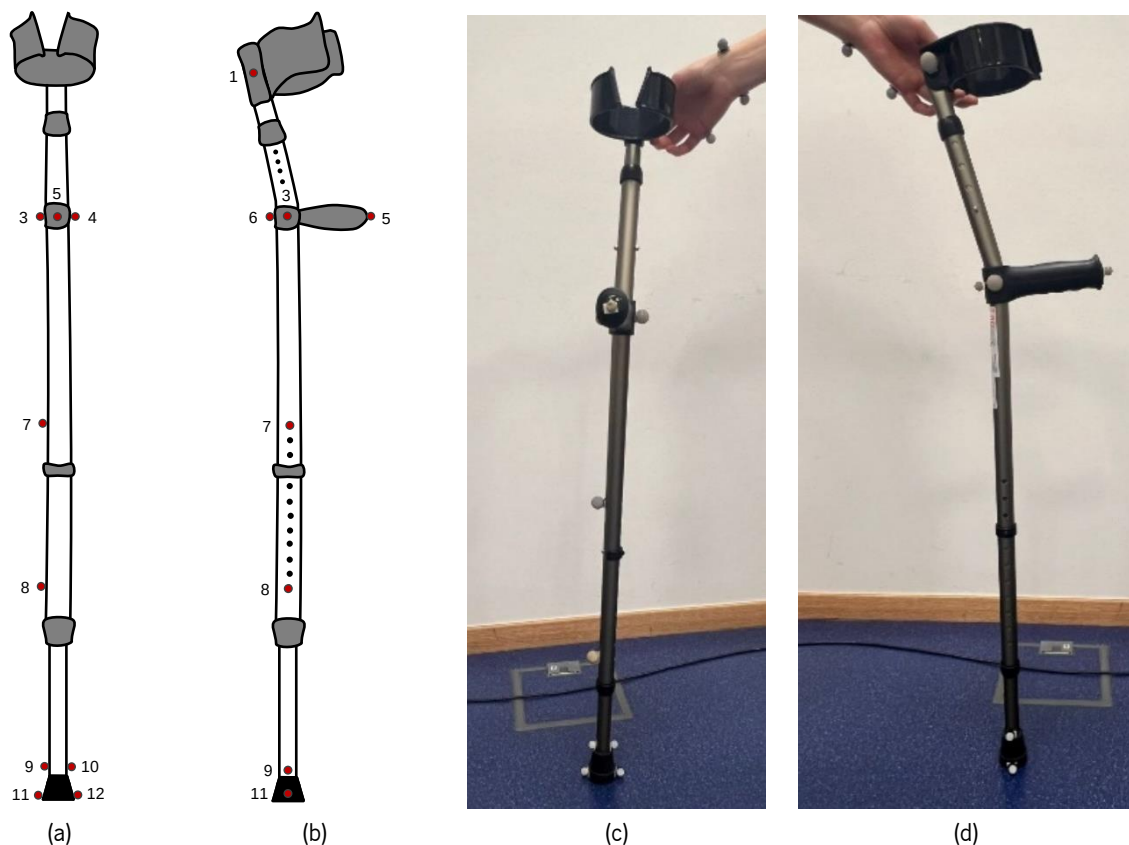


Figure 6.3 – Marker set protocol utilized on the crutches: (a) and (c) front view, and (b) and (d) lateral view.

The surface electromyography (sEMG) activity of the tibialis anterior, soleus and medial and lateral heads of the gastrocnemius was also recorded during the dynamic trials. The placement of the wireless PicoX sensors was also based on the SENIAM project and can be consulted in Figure 5.6.

Prior to the data acquisition procedure, the volunteer had a period of adaptation to the experimental setup. In addition, since the considered volunteer was a healthy subject, this period of adaptation was also utilized to help her become familiar with walking with crutches. During the dynamic trials, the subject was asked to perform four-point crutch-assisted gait. As in the unassisted gait, before each dynamic trial, the subject was instructed to contract the muscles of the legs in order to indicate the beginning of the trial and facilitate the treatment of the sEMG data.

Similarly to the unassisted gait, the duration of each analysis is defined by one complete gait cycle performed by the considered subject, and only gait cycles in which the subject walks from the right to the left x -direction (see Figure 5.7) are considered. The treatment of the trajectory of the markers was initially performed using the Qualisys Track Manager 2.9 (Qualisys©) software and a new Automatic Identification of Markers (AIM) model including the crutches was established. The AIM model contained 91 reflective markers, which represent the 51 markers and the four markers included in each of the four clusters of tracking markers shown in Figure 5.4, as well as the 24 markers of the two crutches, 12 markers placed on each crutch, as depicted in Figure 6.3. The developed AIM model is presented in Figure 6.4, which illustrates the heel strike of the right foot for one trial of crutch-assisted gait. The treated data was then exported to a *.tsv file (table-separated value) to be utilized in MATLAB.

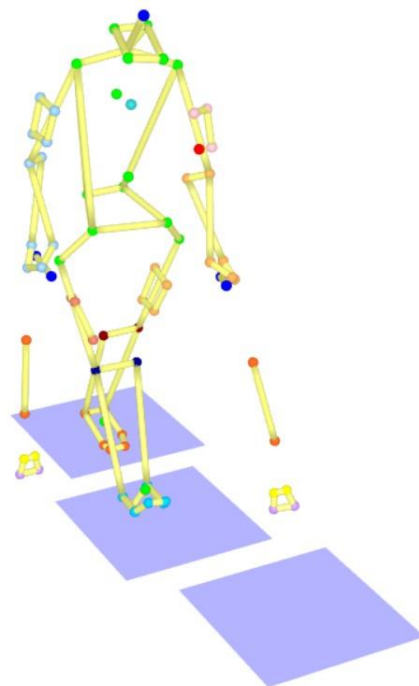


Figure 6.4 – Automatic Identification of Markers (AIM) model developed in the Qualisys Track Manager software to study crutch-assisted gait.

After processing the markers' data in the Qualisys Track Manager software, a third-order low pass digital Butterworth filter with a cutoff frequency of 6 Hz and the zero-phase lag technique were applied in MATLAB. The local reference frame of each crutch was defined as (see Figure 6.3)

$$\zeta = \left\{ \frac{\mathbf{M}_7 - \mathbf{M}_8}{\|\mathbf{M}_7 - \mathbf{M}_8\|} \right\}^T \quad (6.1)$$

$$\mathbf{v}_{aux} = \left\{ \frac{\mathbf{M}_{10} - \mathbf{M}_9}{\|\mathbf{M}_{10} - \mathbf{M}_9\|} \right\}^T \quad (6.2)$$

$$\xi = \tilde{\mathbf{v}}_{aux} \zeta \quad (6.3)$$

$$\eta = \tilde{\zeta} \xi \quad (6.4)$$

The length, mass, moments and products of inertia of the crutches were obtained by consulting the information provided by the CAD model and can be consulted in Table 6.2. The crutch length is considered to be the vertical distance measured from the tip to the top of the cuff.

Table 6.2 – Dimensions and inertial properties of the C8 closed cuff crutch

Length [m]	Mass [kg]	Moments and products of inertia [kg·m ²]					
		$I_{\xi\xi}$	$I_{\eta\eta}$	$I_{\zeta\zeta}$	$I_{\xi\eta}$	$I_{\xi\zeta}$	$I_{\eta\zeta}$
0.9774	0.5290	0.0609830	0.0621187	0.0013849	-0.0000073	-0.0009913	0.0000078

The location of the joint connecting the crutch to the hand with respect to the local coordinates of the connected bodies is presented in Table 6.3. The joint is located at the center of mass of the hand. For the crutch, the joint is considered to be at the handle and its location was obtained by consulting the CAD model. The values relative to the crutch in Table 6.3 are specific to the considered crutch length.

Table 6.3 – Location of the joint connecting the crutch to the hand with respect to the local coordinate systems of each body

Joint	Body	Joint location (right side)			Joint location (left side)		
		ξ [m]	η [m]	ζ [m]	ξ [m]	η [m]	ζ [m]
Hand-Crutch	Hand	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
	Crutch	0.0615	-0.0004	0.1524	0.0615	0.0004	0.1524

The location of the center of mass, Euler parameters, as well as the linear and angular velocities of each crutch were determined using the procedure described in Eqs. (5.37)-(5.45). The matrix $\mathbf{U}$ of Eq. (5.46) was updated to include the two additional bodies, resulting in 260 lines and n time steps. The ground reaction forces (GRF), center of pressure (CoP) and sEMG data were subjected to the treatment procedure described in section 5.3. The kinematic consistency procedure explained in section 5.4 was also considered to guarantee the fulfilment of the kinematic constraints of the model.

6.4. Assistive Device-Model Interface

The modeling process of the interface that exists between the assistive device and the biomechanical multibody model is an important aspect to take into consideration when studying and analyzing device-assisted gait. Since, in this work, forearm crutches are the chosen assistive devices, as explained in sections 2.3 and 6.2, the device-model interface can occur between the crutch handle and the hand, as well as between the crutch cuff and the arm. However, in this work, only the interface between the crutch handle and the hand is addressed since it is at this level that the majority of the load resulting from the interaction that occurs between the crutch and the ground is transmitted to the human body. It is, therefore, a reasonable modeling assumption to disregard the cuff-arm interface.

In this section, two distinct approaches to deal with the interface that exists between the handle of the crutch and the hand of the biomechanical model with the simple shoulder explained in Chapter 5 are compared and discussed. The first approach considers that the hand and the crutch are connected to each other using a fixed joint. This type of kinematic joint was formulated in this work in order to prevent the relative movement between two bodies i and j , thus removing six degrees-of-freedom of the multibody system. Six kinematic constraint equations are formulated for the fixed joint as

$$\Phi^{(f,6)} = \begin{cases} \mathbf{r}_j^P - \mathbf{r}_i^P = \mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i - \mathbf{s}_i^P = \mathbf{0} \\ \mathbf{a}_i^T \mathbf{b}_j - \mathbf{a}_{i,0}^T \mathbf{b}_{j,0} = 0 \\ \mathbf{c}_i^T \mathbf{d}_j - \mathbf{c}_{i,0}^T \mathbf{d}_{j,0} = 0 \\ \mathbf{e}_i^T \mathbf{f}_j - \mathbf{e}_{i,0}^T \mathbf{f}_{j,0} = 0 \end{cases} \quad (6.5)$$

where $\mathbf{r}_k^P$ represents the global position vector of point P located on body k ($k = i, j$), $\mathbf{r}_k$ denotes the global position vector of the center of mass of body k and $\mathbf{s}_k^P$ is the global position vector of point P located on body k with respect to the body's local coordinate system.

The first kinematic constraint of Eq. (6.5) imposes that the geometric center of the fixed joint must have constant coordinates with respect to the local coordinate systems of the connected bodies i and j . This means that point P on body i must be coincident with point P on body j , thus constraining the relative position between the connected bodies. The last three kinematic constraint equations of Eq. (6.5) are considered in order to, in each time step of the analysis, establish a constant orientation between vectors $\mathbf{a}_i, \mathbf{b}_j, \mathbf{c}_i, \mathbf{d}_j, \mathbf{e}_i$ and $\mathbf{f}_j$, and their coordinates in the initial configuration ($\mathbf{a}_{i,0}, \mathbf{b}_{j,0}, \mathbf{c}_{i,0}, \mathbf{d}_{j,0}, \mathbf{e}_{i,0}$ and $\mathbf{f}_{j,0}$). It is important to note that the symbol $\Phi^{(f,6)}$ refers to a fixed (f) joint constraint containing six (6) equations. The observation of Eq. (6.5) leads to the conclusion that the formulation of the fixed joint is based on kinematic constraints that are not explicit functions of time, and, therefore, vector $\mathbf{v}$ is null.

The calculation of the first time derivative of Eq. (6.5) leads to the velocity constraint equations of the proposed fixed joint as

$$\dot{\Phi}^{(f,6)} = \begin{cases} \dot{\mathbf{r}}_j + \dot{\mathbf{s}}_j^P - \dot{\mathbf{r}}_i - \dot{\mathbf{s}}_i^P = \mathbf{0} \\ \mathbf{b}_j^T \dot{\mathbf{a}}_i + \mathbf{a}_i^T \dot{\mathbf{b}}_j = 0 \\ \mathbf{d}_j^T \dot{\mathbf{c}}_i + \mathbf{c}_i^T \dot{\mathbf{d}}_j = 0 \\ \mathbf{f}_j^T \dot{\mathbf{e}}_i + \mathbf{e}_i^T \dot{\mathbf{f}}_j = 0 \end{cases} \quad (6.6)$$

in which the dot represents the derivative with respect to time.

Considering the condition presented in Eq. (3.27), then Eq. (6.6) can be expressed in terms of the angular velocity of bodies i and j as

$$\dot{\Phi}^{(f,6)} = \begin{cases} \dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \dot{\mathbf{r}}_i + \tilde{\mathbf{s}}_i^P \boldsymbol{\omega}_i = \mathbf{0} \\ -\mathbf{b}_j^T \tilde{\mathbf{a}}_i \boldsymbol{\omega}_i - \mathbf{a}_i^T \tilde{\mathbf{b}}_j \boldsymbol{\omega}_j = 0 \\ -\mathbf{d}_j^T \tilde{\mathbf{c}}_i \boldsymbol{\omega}_i - \mathbf{c}_i^T \tilde{\mathbf{d}}_j \boldsymbol{\omega}_j = 0 \\ -\mathbf{f}_j^T \tilde{\mathbf{e}}_i \boldsymbol{\omega}_i - \mathbf{e}_i^T \tilde{\mathbf{f}}_j \boldsymbol{\omega}_j = 0 \end{cases} \quad (6.7)$$

where the symbol tilde ($\sim$) represents the skew symmetric matrix associated with that vector, and $\boldsymbol{\omega}$ is the angular velocity vector in global coordinates.

Therefore, the contribution of the fixed joint to the Jacobian matrix can be defined as

$$\mathbf{D}^{(f,6)} = \begin{bmatrix} -\mathbf{I} & \tilde{\mathbf{s}}_i^P & \mathbf{I} & -\tilde{\mathbf{s}}_j^P \\ \mathbf{0} & -\mathbf{b}_j^T \tilde{\mathbf{a}}_i & \mathbf{0} & -\mathbf{a}_i^T \tilde{\mathbf{b}}_j \\ \mathbf{0} & -\mathbf{d}_j^T \tilde{\mathbf{c}}_i & \mathbf{0} & -\mathbf{c}_i^T \tilde{\mathbf{d}}_j \\ \mathbf{0} & -\mathbf{f}_j^T \tilde{\mathbf{e}}_i & \mathbf{0} & -\mathbf{e}_i^T \tilde{\mathbf{f}}_j \end{bmatrix} \quad (6.8)$$

in which $\mathbf{I}$ is the identity matrix.

Finally, by taking the first time derivative of Eq. (6.6), the acceleration constraint equations of the fixed joint can be established as

$$\ddot{\Phi}^{(f,6)} = \begin{cases} \ddot{\mathbf{r}}_j + \ddot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i - \ddot{\mathbf{s}}_i^P = \mathbf{0} \\ \mathbf{b}_j^T \ddot{\mathbf{a}}_i + \dot{\mathbf{a}}_i^T \dot{\mathbf{b}}_j + \mathbf{a}_i^T \ddot{\mathbf{b}}_j + \dot{\mathbf{b}}_j^T \dot{\mathbf{a}}_i = 0 \\ \mathbf{d}_j^T \ddot{\mathbf{c}}_i + \dot{\mathbf{c}}_i^T \dot{\mathbf{d}}_j + \mathbf{c}_i^T \ddot{\mathbf{d}}_j + \dot{\mathbf{d}}_j^T \dot{\mathbf{c}}_i = 0 \\ \mathbf{f}_j^T \ddot{\mathbf{e}}_i + \dot{\mathbf{e}}_i^T \dot{\mathbf{f}}_j + \mathbf{e}_i^T \ddot{\mathbf{f}}_j + \dot{\mathbf{f}}_j^T \dot{\mathbf{e}}_i = 0 \end{cases} \quad (6.9)$$

Taking advantage of Eq. (3.31), then Eq. (6.9) can be expressed in terms of the angular accelerations of bodies i and j , yielding the following expression

$$\ddot{\Phi}^{(f,6)} = \begin{cases} \ddot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i + \tilde{\mathbf{s}}_i^P \dot{\boldsymbol{\omega}}_i - \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_i^P = \mathbf{0} \\ \mathbf{b}_j^T (-\tilde{\mathbf{a}}_i \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{a}}_i) + \dot{\mathbf{a}}_i^T \dot{\mathbf{b}}_j + \mathbf{a}_i^T (-\tilde{\mathbf{b}}_j \dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{b}}_j) + \dot{\mathbf{b}}_j^T \dot{\mathbf{a}}_i = 0 \\ \mathbf{d}_j^T (-\tilde{\mathbf{c}}_i \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{c}}_i) + \dot{\mathbf{c}}_i^T \dot{\mathbf{d}}_j + \mathbf{c}_i^T (-\tilde{\mathbf{d}}_j \dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{d}}_j) + \dot{\mathbf{d}}_j^T \dot{\mathbf{c}}_i = 0 \\ \mathbf{f}_j^T (-\tilde{\mathbf{e}}_i \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{e}}_i) + \dot{\mathbf{e}}_i^T \dot{\mathbf{f}}_j + \mathbf{e}_i^T (-\tilde{\mathbf{f}}_j \dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{f}}_j) + \dot{\mathbf{f}}_j^T \dot{\mathbf{e}}_i = 0 \end{cases} \quad (6.10)$$

where $\dot{\boldsymbol{\omega}}$ is the angular acceleration vector in global coordinates.

Hence, the contribution of Eq. (6.5) to the right-hand side of the acceleration equations yields

$$\gamma^{(f,6)} = \begin{Bmatrix} -\tilde{\omega}_j \dot{\mathbf{s}}_j^P + \tilde{\omega}_i \dot{\mathbf{s}}_i^P \\ -\mathbf{b}_j^T \tilde{\omega}_i \dot{\mathbf{a}}_i - \mathbf{a}_i^T \tilde{\omega}_j \dot{\mathbf{b}}_j - 2\dot{\mathbf{a}}_i^T \dot{\mathbf{b}}_j \\ -\mathbf{d}_j^T \tilde{\omega}_i \dot{\mathbf{c}}_i - \mathbf{c}_i^T \tilde{\omega}_j \dot{\mathbf{d}}_j - 2\dot{\mathbf{c}}_i^T \dot{\mathbf{d}}_j \\ -\mathbf{f}_j^T \tilde{\omega}_i \dot{\mathbf{e}}_i - \mathbf{e}_i^T \tilde{\omega}_j \dot{\mathbf{f}}_j - 2\dot{\mathbf{e}}_i^T \dot{\mathbf{f}}_j \end{Bmatrix} \quad (6.11)$$

The second approach utilized to deal with the interface between the crutch and the model substitutes the fixed joint by a geometrically ideal spherical joint. The spherical joint is formulated using the first line only of Eqs. (6.5)-(6.11) and it constrains three relative translations and allows three relative rotations of the bodies that it connects, yielding three degrees-of-freedom (M. R. Silva et al., 2022a). In both approaches, the crutch is added to the biomechanical multibody model as an independent rigid body. Therefore, the number of bodies increases to 20, as opposed to the 18 bodies established in section 5.1. This type of modeling approach for introducing the crutches into the model has been previously reported by several authors and can be consulted in Table 2.5 and Figure 2.7 of the literature review presented in section 2.3. It is important to note that, while the crutch is considered an independent body of the model, since there is no relative movement between the hand and the crutch in the fixed joint approach, meaning that these two bodies are rigidly connected to each other, in reality, this case is equivalent to considering the crutch-hand as a unique body or the crutch as an extension of the hand (see Table 2.5 and Figure 2.7). It must be stated that, amongst the 25% of studies modeling the crutch-body as a unique rigid body in Figure 2.7, none has considered the hand for this purpose.

Since no relative movement between the bodies i and j connected by the joint is allowed when the fixed joint approach is considered, the number of degrees-of-freedom of the biomechanical multibody model remains the same as the one determined in section 5.1, that is, 39 degree-of-freedom. In turn, when the spherical joint approach is utilized to deal with the device-model interface, since relative movement between the connected bodies can occur, the number of degrees-of-freedom of the model is updated to 45, which includes three additional degrees-of-freedom for each crutch.

The point chosen for the interface that occurs between the handle of the crutch and the hand of the biomechanical multibody model is denoted as point P . In both approaches, the following assumptions are taken into consideration: (i) point P on the hand is located on its center of mass and (ii) point P on the crutch is located on its handle. For the fixed joint approach, it is also considered that the orientation of the hand relative to the crutch is constant during the entire analysis and it is equal to the orientation in the first instant of time. For the spherical joint approach, three independent degrees-of-freedom exist between the connected bodies. Figure 6.5 presents a representation of point P on the crutch and hand.

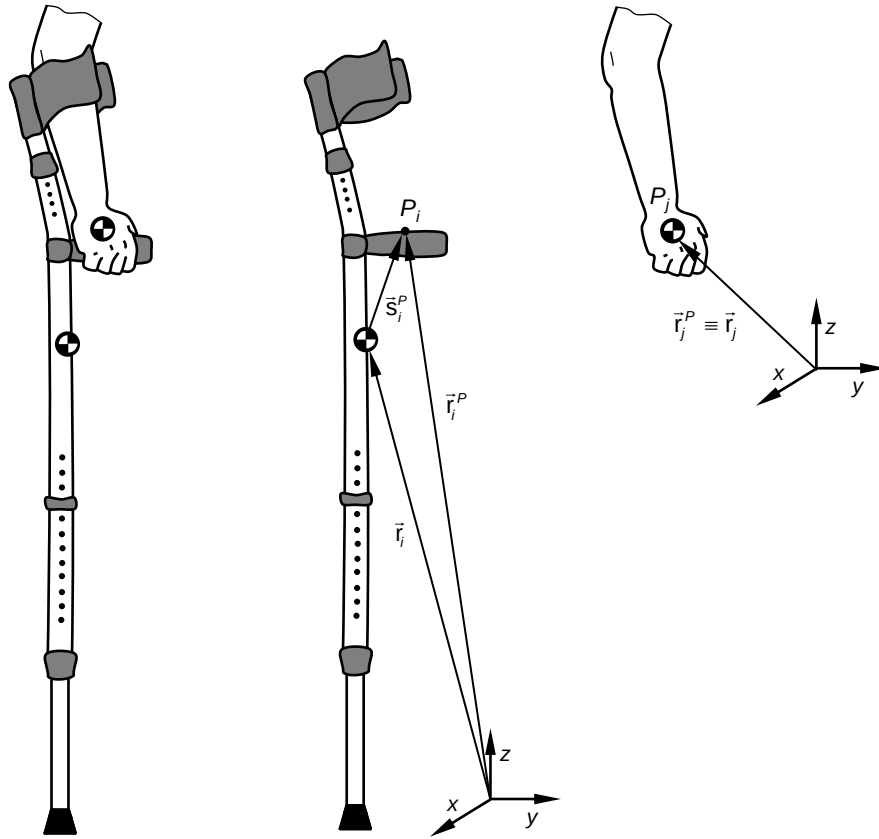


Figure 6.5 – Schematic representation of the point P chosen for the crutch-model interface. It is assumed that the crutch is the body i and the hand is the body j .

Figure 6.6 presents a representation of the biomechanical model incorporated with crutches.

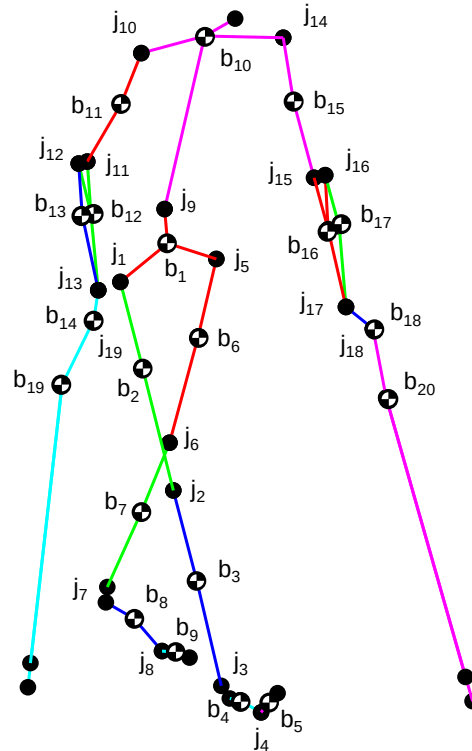


Figure 6.6 – Configuration of the biomechanical multibody model with the simple shoulder and crutches.

In this section, the four-point reciprocal crutch-assisted gait pattern is considered in order to compare the two approaches utilized to deal with the interface between the handle and the model. The gait cycle begins and ends with the heel strike of the right foot. In the beginning of the analysis both feet and crutches are in contact with the ground. The considered gait sequence begins with the right foot in contact with force plate 2, followed by the contact of the right crutch with the ground. The left foot then contacts the force plate 3 and, afterwards, the left crutch contacts the ground. Figure 6.7 presents the snapshots of the gait sequence in the Qualisys Track Manager software.

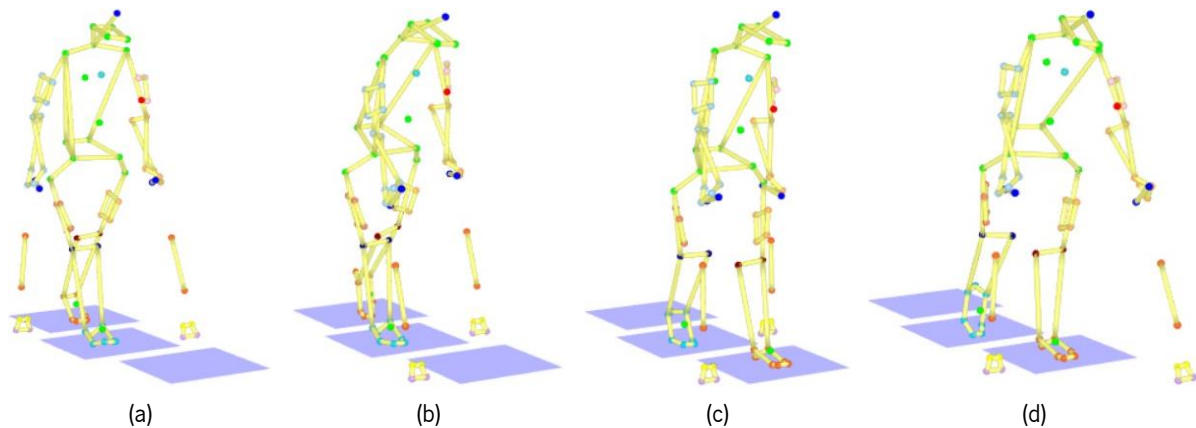


Figure 6.7 – Snapshots of the Automatic Identification of Markers (AIM) model performing four-point reciprocal crutch-assisted gait in the Qualisys Track Manager software. Gait sequence: (a) right foot, (b) right crutch, (c) left foot, and (d) left crutch.

As explained in section 5.4, the processed experimental data of the recorded movement does not guarantee that the kinematic constraints associated with the biomechanical model are fulfilled. In order to overcome this issue, a kinematic consistency procedure must be employed. The constraint equations considered in Eq. (5.50) of the referred consistency procedure are those associated with the formulation of the joints of the model, specifically the spherical, revolute, universal, body-followed and fixed joints (see Table 5.1). Therefore, Eq. (5.50) indicates that the corrected and kinematically consistent coordinates of the multibody model are influenced by the uncorrected coordinates arising from the processed experimental data, as well as by the kinematic constraints imposed by the joints. In this work, the location of the center of mass of each body utilized in the vector of the uncorrected coordinates is achieved by using a sequential process, in which the center of mass of the lower trunk, i.e., the parent body, is located based on four markers and then the location of the center of mass of the subsequent bodies is found by using the vectors locating the joint relative to the body. This process is explained in detail in Eqs. (5.37) and (5.38). An alternative approach to the sequential process could be to, first, locate the joint using the experimental data of the markers and subtracting the vector locating the joint relative to the body in order to find the center of mass of the body. An example of the alternative process for locating the center of mass of the right leg is expressed by the following condition (see Figure 5.4)

$$\mathbf{r}_{leg} = \frac{\mathbf{M}_{30} + \mathbf{M}_{32}}{2} - \mathbf{s}_{leg}^{knee} \quad (6.12)$$

in which $\mathbf{r}_{leg}$ represents the global position vector of the center of mass of the leg, $\mathbf{M}_{30}$ and $\mathbf{M}_{32}$ denote markers placed on the lateral and medial aspects of the knee (see Figure 5.4), respectively, and $\mathbf{s}_{leg}^{knee}$ is the global position vector of the knee joint located on the leg with respect to its local coordinate system.

The use of the sequential approach might be prone to inaccuracies, which are larger the further away from the parent body the estimation of the center of mass of the other bodies is made. In this work, it was noticed that the trajectory of the z -coordinate of the tip of the crutch calculated using the sequential approach presented significant differences when compared with the trajectory of the midpoint between the markers located on the crutch tip, i.e., $\mathbf{M}_{11}$ and $\mathbf{M}_{12}$ of Figure 6.3. In order to correct this problem, the implemented solution was to, in the kinematic consistency procedure, besides calculating the corrected coordinates of the model based on the uncorrected coordinates and constraints imposed by the joints only, six driving constraints for each crutch were also added. These constraints were utilized to guide the trajectory of the center of mass of each crutch using Eqs. (3.67)-(3.74), as well as the orientation of the crutches using Eqs. (3.75)-(3.81). The determination of the Euler parameters of each crutch followed the same procedure as the one described in Eqs. (5.39)-(5.44). Hence, for the calculation of the center of mass of the crutch, the alternative approach was utilized as (see Figure 6.3)

$$\mathbf{r}_{crutch} = \frac{\mathbf{M}_{11} + \mathbf{M}_{12}}{2} - \mathbf{s}_{crutch}^{tipM} \quad (6.13)$$

where $\mathbf{r}_{crutch}$ denotes the global position vector of the center of mass of the crutch, $\mathbf{M}_{11}$ and $\mathbf{M}_{12}$ are markers placed on the lateral and medial aspects of the crutch tip (see Figure 6.3) and $\mathbf{s}_{crutch}^{tipM}$ represents the global position vector of the midpoint between the markers on the crutch tip joint located on the crutch with respect to the local coordinate system of the crutch. The sequential approach was utilized for the calculation of the location of the center of mass of all bodies of the model, except for the crutches.

Figure 6.8a shows the trajectory of the z -coordinate of the tip of the right crutch determined using the sequential and alternative approaches, and the midpoint between the markers $\mathbf{M}_{11}$ and $\mathbf{M}_{12}$ of Figure 6.3, while Figure 6.8b presents a schematic representation of the location of the points of interest in this analysis. The use of the sequential approach provides significantly different results when compared with the midpoint between the markers. In turn, the alternative approach produces a curve for the z -coordinate of the tip closer to the markers' data. It should be noted that the midpoint M between markers $\mathbf{M}_{11}$ and $\mathbf{M}_{12}$ is placed above the point T considered for the crutch tip (see Figure 6.8b), which explains the offset observed between the red and green plots of Figure 6.8a. The results for the left crutch are identical.

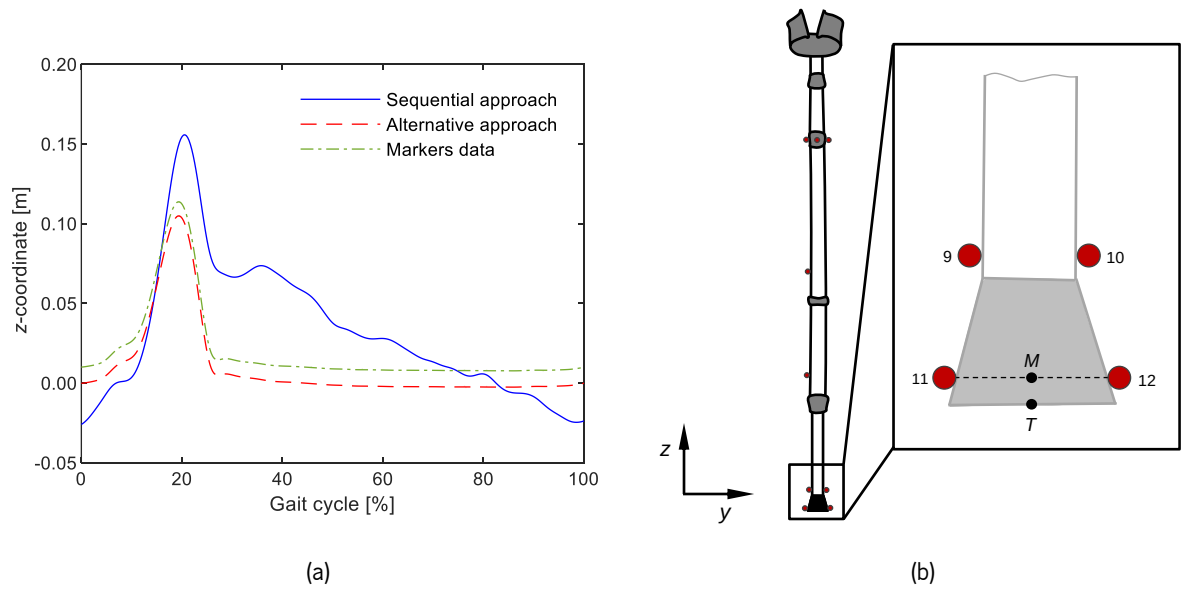


Figure 6.8 – (a) Trajectory of the z -coordinate of the right crutch tip (blue and red plots) and midpoint between the tip markers (green plot). A comparison between the sequential approach, alternative approach and midpoint between the crutch markers is provided. (b) Schematic representation of the midpoint M between the $\mathbf{M}_{11}$ and $\mathbf{M}_{12}$ markers and point T located on the tip.

Figure 6.9 provides a comparison between the fixed and spherical joint approaches, and depicts the z -coordinate of the center of mass of the right crutch, hand and radius, as well as the z -coordinate of the radiocarpal joint throughout the gait cycle. It can be observed that there are no significant differences in the crutch and hand plots, which is sound because (i) the trajectory of the center of mass of the crutch is estimated similarly for both approaches using the modification in the kinematic consistency procedure explained in the previous paragraphs, and (ii) point P is located on the center of mass of the hand. If the point of interface between the crutch and the model would be any other point with the exception of the center of mass of the hand, then there would be differences between both approaches. It can also be observed that the trajectory of the center of mass of the radius differs between both approaches. This result is associated with the fact that, since the trajectory of the center of mass of the crutch is forced to be followed using the point and Euler parameters driving constraints in the modified kinematic consistency procedure, the trajectory of all the other elements defined prior the hand, i.e. radiocarpal joint, radius, ulna, and the other bodies and joints, must be adjusted in order to account for the existence or absence of relative movement between the hand and the crutch. In the spherical joint case, three independent degrees-of-freedom exist between the connected bodies, which leads to a movement of the biomechanical model closer to the reality. This can be confirmed from the fact that, in Figure 6.9d, the z -coordinate of the radiocarpal joint estimated using the spherical joint approach is closer to the trajectory of the same joint calculated as the midpoint between markers $\mathbf{M}_{16}$ and $\mathbf{M}_{18}$ of Figure 5.4. The conclusions drawn out in this paragraph allow to justify the choice of the spherical joint approach to deal with the crutch-model interface in the analyses carried out in the following sections.

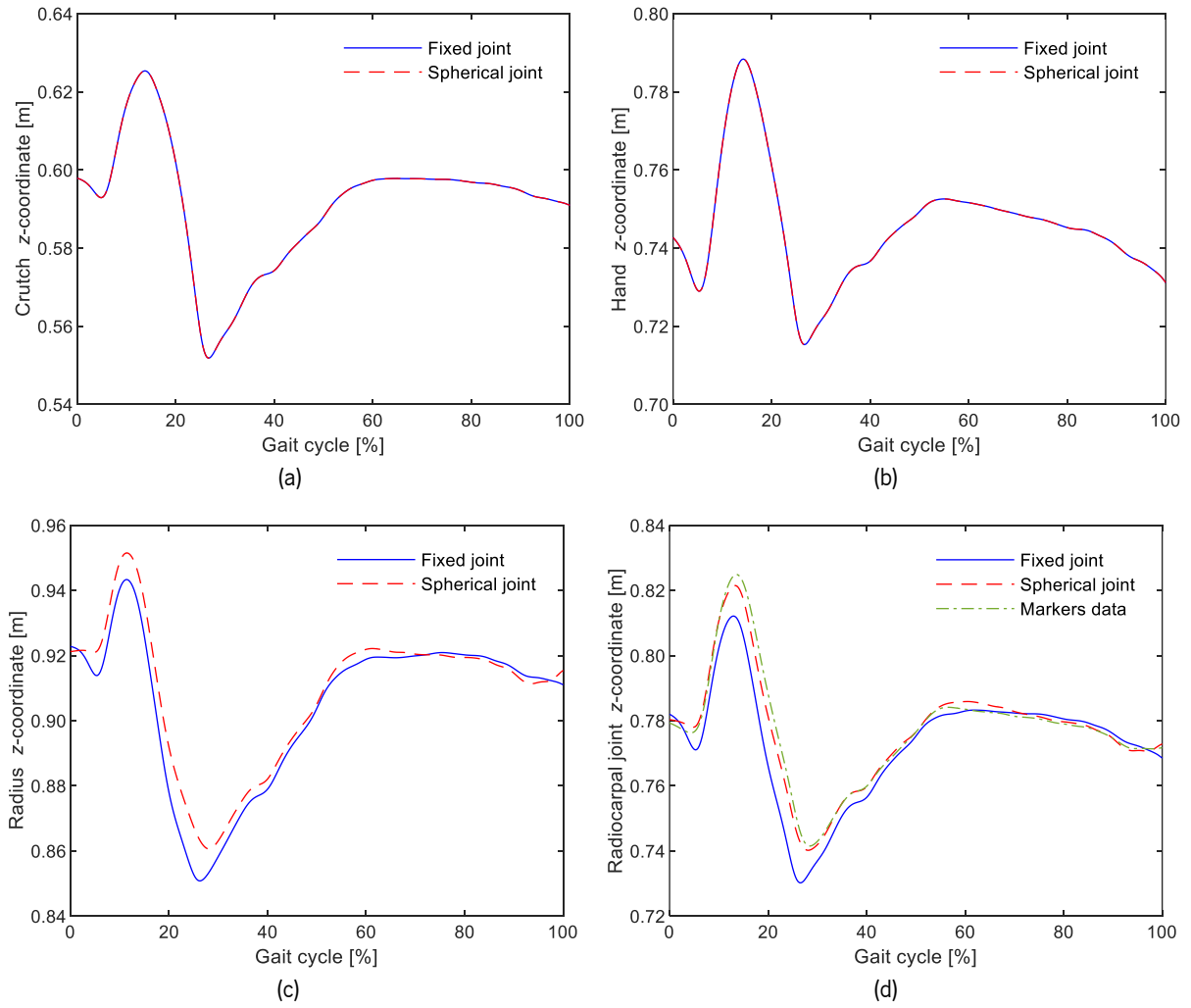


Figure 6.9 – Trajectory of the z-coordinate of the center of mass of the right (a) crutch, (b) hand and (c) radius, and (d) trajectory of the z-coordinate of the right radiocarpal joint. A comparison between the fixed and spherical joint approaches utilized to deal with the crutch-model interface is provided. The midpoint between the $\mathbf{M}_{16}$ and $\mathbf{M}_{18}$ markers is also considered.

6.5. Assistive Device-Ground Interface

Accurate modeling of the interface that exists between the assistive device and the ground, as well as obtaining close to reality results are critical and challenging processes that have not been approached in depth yet. Therefore, the objective of this section is to develop a computational model of the crutch-ground interface and compare the obtained results with the experimental data acquired at the Lisbon Biomechanics Laboratory.

In this work, the sphere-plane contact detection algorithm is chosen and implemented in the in-house code MUBODYNA, a procedure which is in accordance with the methodologies followed by two studies identified and analyzed in the literature review presented in section 2.3 (Febrer-Nafria et al., 2021; Font-Llagunes et al., 2012). The crutch tip is considered to be a sphere i with geometric center located

on point C and radius R . In turn, the ground is assumed to be a plane j defined by a point G and a normal unit vector $\mathbf{n}_j$. A schematic representation of the interface existing between the crutch and the ground established as a sphere-plane geometrical condition is provided in Figure 6.10.

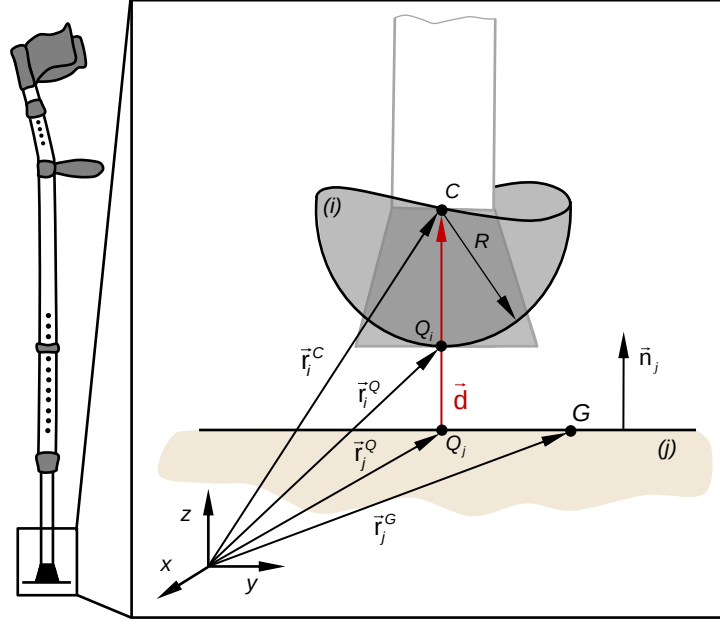


Figure 6.10 – Schematic representation of the interface existing between the crutch and the ground.

The distance from the center of the sphere to the plane, d , can be calculated by the following expression (Gismeros Moreno et al., 2024)

$$d = \mathbf{n}_j^T (\mathbf{r}_i^C - \mathbf{r}_j^G) \quad (6.14)$$

where $\mathbf{r}_i^C$ and $\mathbf{r}_j^G$ are the global position vectors of points C and G on bodies i and j , respectively.

The vector $\mathbf{d}$ observed in Figure 6.10 can be defined as

$$\mathbf{d} = d\mathbf{n}_j \quad (6.15)$$

The projection of the center of the sphere i on the plane j determines the potential point of contact Q in the plane. The coordinates of the contact point on the plane, Q , are calculated by

$$\mathbf{r}_j^Q = \mathbf{r}_i^C - \mathbf{d} \quad (6.16)$$

In turn, the coordinates of the contact point on the sphere, Q , can be estimated as

$$\mathbf{r}_i^Q = \mathbf{r}_i^C - R\mathbf{n}_j \quad (6.17)$$

At this point, it is, therefore, possible to establish the expression for the calculation of the penetration, δ , between both surfaces as

$$\delta = R - d \quad (6.18)$$

A positive value for the penetration indicates the occurrence of contact between the sphere and the plane. In this situation, the velocities of the contact points Q on the plane and on the sphere must be determined and are evaluated, respectively, as

$$\dot{\mathbf{r}}_j^Q = \dot{\mathbf{r}}_j + \tilde{\boldsymbol{\omega}}_j (\mathbf{r}_j^Q - \mathbf{r}_j) \quad (6.19)$$

$$\dot{\mathbf{r}}_i^Q = \dot{\mathbf{r}}_i + \tilde{\boldsymbol{\omega}}_i (\mathbf{r}_i^Q - \mathbf{r}_i) \quad (6.20)$$

Equations (6.19)-(6.20) are obtained by taking the first time derivative of the following condition

$$\mathbf{r}_k^Q = \mathbf{r}_k + \mathbf{s}_k^Q \quad (6.21)$$

where $\mathbf{r}_k^Q$ represents the global position vector of the contact point Q located on body k , $\mathbf{r}_k$ denotes the global position vector of the center of mass of body k and $\mathbf{s}_k^Q$ is the global position vector of the contact point Q located on body k with respect to the body's local coordinate system.

The relative normal, $\mathbf{v}_n$, and tangential, $\mathbf{v}_t$, velocities of the contact points Q determine whether the bodies in contact are approaching or separating, and whether they are sliding or sticking, respectively. The relative velocities are obtained by projecting the relative contact velocity onto the normal and tangential directions as

$$\mathbf{v}_n = \left[(\dot{\mathbf{r}}_i^Q - \dot{\mathbf{r}}_j^Q)^T \mathbf{n}_j \right] \mathbf{n}_j \quad (6.22)$$

$$\mathbf{v}_t = (\dot{\mathbf{r}}_i^Q - \dot{\mathbf{r}}_j^Q) - \mathbf{v}_n \equiv v_t \mathbf{t} \quad (6.23)$$

where v_t is the magnitude of the relative tangential velocity and $\mathbf{t}$ is the tangential direction of the relative velocity associated with the contacting surfaces represented as

$$\mathbf{t} = \frac{\mathbf{v}_t}{v_t} \quad (6.24)$$

The dynamics of the sphere-plane contact phenomenon is controlled by contact-impact forces arising from the interaction between the connected bodies. In contact mechanics, the evaluation of normal and tangential contact forces resulting from collisions between bodies is an aspect of utmost importance to take into consideration. In this work, the normal contact force vector, $\mathbf{f}_n$, is evaluated by using the Hunt and Crossley contact force model (Hunt & Crossley, 1975), as implemented in another study in this area of investigation (Font-Llagunes et al., 2012)

$$\mathbf{f}_n = (K\delta^n + \chi\delta^n\dot{\delta})\mathbf{n}_j \quad (6.25)$$

in which K is the generalized contact stiffness, n denotes the nonlinear exponent factor, δ is the penetration calculated in Eq. (6.18), χ is the hysteresis damping factor and $\dot{\delta}$ is the penetration velocity.

The generalized stiffness parameter is dependent on the material properties and on the local geometry of the contacting surfaces. For a sphere i and a plane j in contact, the parameter is computed based on the radius of the sphere, as well as on the material properties of the sphere and the plane as

$$K = \frac{4}{3(\sigma_i + \sigma_j)} \sqrt{R} \quad (6.26)$$

where the material properties σ_i and σ_j are given by

$$\sigma_k = \frac{1 - \nu_k^2}{E_k} \quad (k = i, j) \quad (6.27)$$

in which the quantities ν_k and E_k represent the Poisson's ratio and the Young's modulus associated with the sphere i and the plane j , respectively.

According to Hunt & Crossley (1975), the hysteresis damping factor presented in Eq. (6.25) can be expressed by the following condition

$$\chi = \frac{3(1 - c_r)}{2} \frac{K}{\dot{\delta}^{(-)}} \quad (6.28)$$

where c_r is the coefficient of restitution and $\dot{\delta}^{(-)}$ is the penetration velocity at the beginning of the contact.

In this section, the four-point reciprocal crutch-assisted gait pattern is also considered. As explained in section 6.4, in the beginning of the analysis, both feet and both crutches are in contact with the ground (see Figure 6.7). In this situation, it is not possible to determine the velocity at the beginning of the contact and, therefore, the hysteresis damping factor cannot be dependent on $\dot{\delta}^{(-)}$ (Poursina & Nikravesh, 2024). Consequently, since the impact velocities between the crutch and the ground are similar throughout the entire analysis, the same value for the hysteresis damping factor is considered in all contacts, following the procedures carried out in a previous study (Font-Llagunes et al., 2012).

A substantial number of friction force models that can be used in the context of multibody systems formulations are available in the literature, and they might be classified as static or dynamic models (Marques et al., 2016). The steady-state behavior of the friction force-relative velocity relation is usually considered in the static models, making them easier to implement in multibody codes. The second group of friction models, the dynamic ones, illustrates the friction phenomena more realistically since extra state variables are considered in the formulation, providing additional degrees-of-freedom for each frictional contact (Marques et al., 2016, 2019).

In the model presented by Threlfall (1978), which is a static tangential force model, an exponential function relates the friction force and the tangential velocity. This model was the starting point

for the development of other friction force models, such as the continuous function that is utilized in this work in order to evaluate the friction force. The continuous function has also been utilized by other study in this area of investigation (Febrer Nafria, 2020). The tangential force, $\mathbf{f}_t$, using the continuous function is expressed as (M. R. Silva et al., 2022a)

$$\mathbf{f}_t = f_c \tanh\left(\frac{v_t}{v_1}\right) \mathbf{t} \quad (6.29)$$

where v_1 is the threshold for the velocity and f_c is the magnitude of the Coulomb's friction denoted as

$$f_c = \mu_k f_n \quad (6.30)$$

in which μ_k is the kinetic coefficient of friction, and f_n represents the normal contact force magnitude.

During the experimental data acquisition at the Lisbon Biomechanics Laboratory, the reaction forces between the crutch tip and the ground during crutch-assisted gait were also recorded using the force plates. In this situation, due to the fact that only three force plates were available, only one foot and one crutch contacted the plates, as observed in Figure 6.11. This procedure was conducted in order to provide an estimation of the crutch-ground reaction forces, which ultimately would allow a comparison and critical analysis with the results provided by the sphere-plane contact detection algorithm.

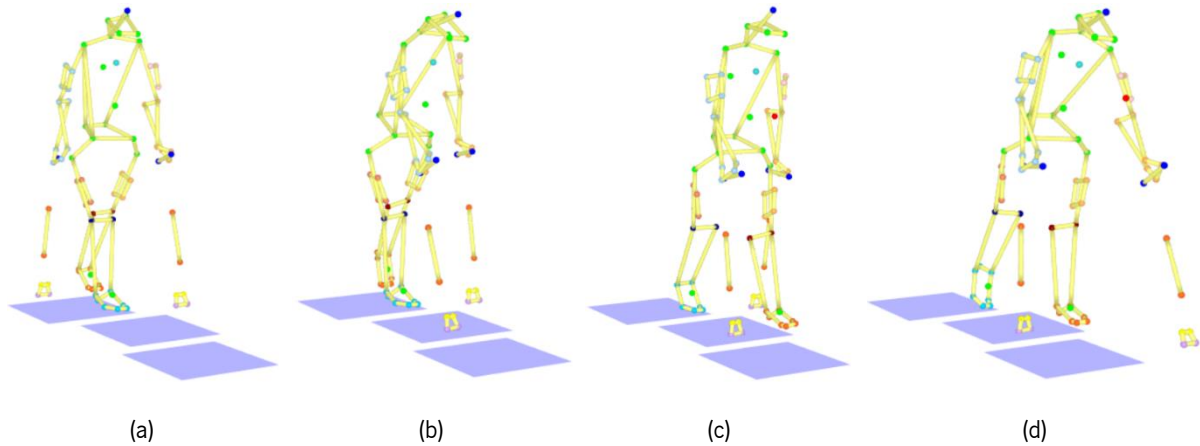


Figure 6.11 – Snapshots of the Automatic Identification of Markers (AIM) model performing four-point reciprocal crutch-assisted gait in the Qualisys Track Manager software with measurement of the reaction forces between the crutch tip and the ground using the force plates. Gait sequence: (a) right foot, (b) right crutch, (c) left foot, and (d) left crutch.

The Young's modulus and Poison's ratio for the ground were taken from Font-Llagunes et al. (2012), which established concrete as the material for this element. The radius of the sphere was considered to be the height of the crutch tip (see Figure 6.2 and Figure 6.10) and was measured from the CAD model discussed in section 6.2. The Poison's ratio of the sphere was also taken from the CAD model, considering the PVC as the material of the crutch tip. In an initial approach, the Young's modulus of the sphere was also taken from the CAD model with a value of 2.76×10^9 Pa. However, it was noted

that the resulting normal contact force presented higher magnitudes than expected for this application case and higher than the magnitudes measured in the laboratory using the procedures described in Figure 6.11. Hence, the Young's modulus of the sphere was adjusted based on the information contained in the datasheet of the crutch tip material provided by ORTHOS XXI and using a trial-and-error approach until the magnitude of the normal contact force resulting from the simulation matched that of the experimental data, resulting in a value of 2.45×10^6 Pa. Using the condition expressed in Eq. (6.26) and the information present in Table 6.4, the generalized contact stiffness yields a value of 8.52×10^5 N/m^{1.5}. In addition, the ratio between the generalized contact stiffness and the hysteresis damping factor calculated from the parameters provided in the study of Font-Llagunes et al. (2012) was utilized to determine the hysteresis damping factor that should be utilized in this work, which resulted in a value of 2.15×10^5 Ns/m^{1.5}. The kinetic friction coefficient was obtained by trial-and-error approach, which purpose was to match the magnitude of the experimental friction forces. A value of 1.00 is utilized, which is equal to the coefficient used by Febrer-Nafria et al. (2021). The contact parameters are shown in Table 6.4.

Table 6.4 – Contact parameters used in the dynamic simulation of the sphere-plane contact

Geometrical and Material Parameters				
Sphere			Plane	
Radius [mm]	Young's modulus [Pa]	Poisson's ratio [-]	Young's modulus [Pa]	Poisson's ratio [-]
48	2.45×10^6	0.40	3.00×10^{10}	0.20
Contact Force Model Parameters				
Kinetic coefficient of friction [-]	Velocity threshold [m/s]	Nonlinear exponent [-]	Hysteresis damping factor [Ns/m ^{1.5}]	
1.00	0.05	1.50	2.15×10^5	

Figure 6.12 depicts the evolution of the penetration throughout the gait cycle calculated using Eq. (6.18) of the sphere-plane contact algorithm for the right and left crutches. It can be concluded that the profile of the plot is in accordance with the periods of the contact between each crutch and the ground for the experimental trial under analysis, that is, the four-point reciprocal gait depicted in Figure 6.7 (gait sequence: right foot, right crutch, left foot, and left crutch). As stated previously, the analysis starts with both feet and both crutches in contact with the ground (see Figure 6.7), which is consistent with the results obtained in Figure 6.12 for the beginning of the gait cycle due to the fact that there is some level of penetration for both crutches. Then, while the left crutch and both feet are still contacting the ground from approximately 1-30% of the gait cycle, the right crutch loses contact with the ground and, consequently, the associated penetration is null. From 30-55% of the gait cycle, while the left foot advances, both crutches and the right foot are in contact with the ground, which agrees with the

calculation of penetration for both crutches. From 55-75% of the gait cycle, the left crutch does not contact the ground and the corresponding penetration is null. The gait cycle ends with both crutches and both feet contacting the ground, which explains the penetration observed in the last part of Figure 6.12. It is also important to mention that the obtained magnitude for the penetration is within acceptable values concerning the sensitivity of the infrared cameras utilized at the Lisbon Biomechanics Laboratory. The error associated with the measurement of the motion capture system is around 1 mm, which represents more than 20% of the maximum value obtained in Figure 6.12 for the penetration. Since the cameras are placed far away from the crutch markers, there is some degree of uncertainty associated with the measurement of their coordinates and, therefore, it is not possible to capture the deformations experienced by the material of the crutch tip with sufficient accuracy to obtain close to reality results for the penetration. While this might not be an issue for the estimation of the large motion associated with the anatomical segments, in contact problems, the relative motion between the contacting surfaces has a very narrow range, mainly in the normal direction. The above-mentioned uncertainty might lead to significant errors on the estimation of the penetration, and, consequently, on the determination of the normal and tangential contact forces. Moreover, in Figure 6.12, it can also be observed that the magnitude of the penetration for the left crutch is higher than that obtained for the right crutch. These results might be attributed to the error accumulated on the motion capture system as the distance from the crutch markers to the cameras increases, resulting in larger errors.

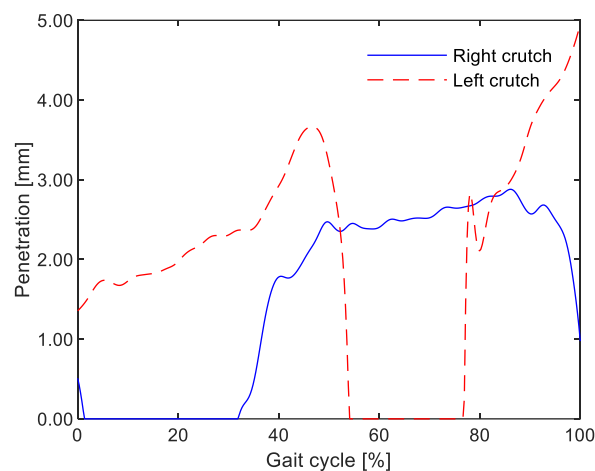
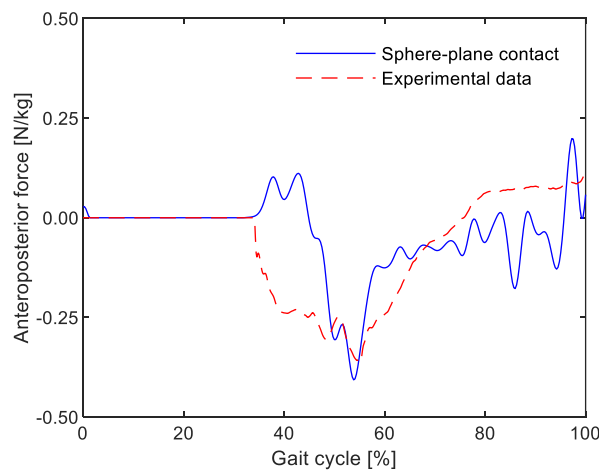


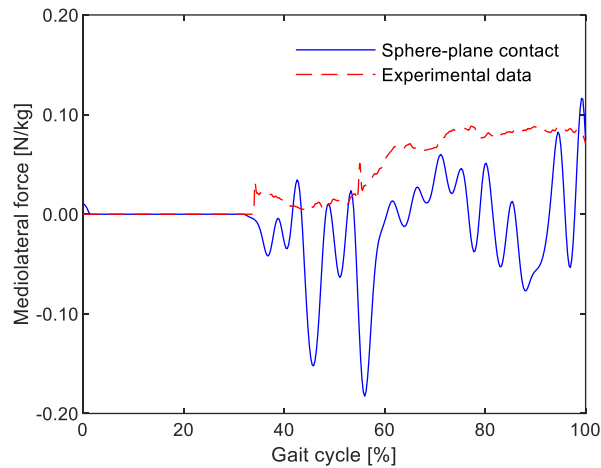
Figure 6.12 – Comparison of the penetration calculated from the sphere-plane contact algorithm for the right and left crutches.

Figure 6.13 compares the crutch-ground reaction forces resulting from the sphere-plane contact detection algorithm and data acquired at the laboratory. It is important to note that the forces from the algorithm were estimated using the trial presented in Figure 6.7, that is, without the experimental measurement of the contact forces. In turn, the forces resulting from the experimental data were acquired

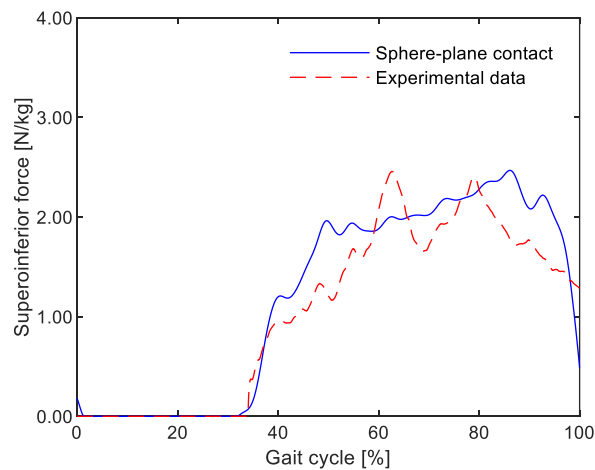
using the trial depicted in Figure 6.11. Therefore, it must be mentioned that a comparison between two different trials is done in Figure 6.13. Although the trials were performed on the same day, with the same marker set protocol and with the same subject, the results are not completely comparable, and caution should be taken when analyzing them and drawing out conclusions. However, the comparison allows to validate the contact algorithm in terms of magnitude and shape of the curves to a certain extent. Concerning the anteroposterior and mediolateral friction forces depicted in Figure 6.13a and Figure 6.13b, the magnitude and profile of the plots obtained with the contact algorithm show similar tendencies to those observed in the experimental data, but the results are not satisfactory. In turn, the superior/inferior or normal contact force (see Figure 6.13c) shows good agreement when compared with the experimental data, both in magnitude and profile of the plot. It is, therefore, evident that the curves obtained for the friction force should be improved in order to obtain similar results to those of the normal force when compared with the experimental data. However, it is known that the stick-slip phenomenon is a major issue for the modeling and simulation of mechanical systems, since it is unstable and not easy to predict. Additionally, the choice of the friction model is of utmost importance as it must be capable of capturing the behavior of the friction force and its influence on the dynamics of the system (Marques et al., 2016). Hence, it is important to note that, during crutch-ground contact, only stick occurs and the model of Eq. (6.29) may not be able to reproduce the magnitude and profile of the force. Observing the experimental curve, the magnitude of the friction force is around 4-15% the magnitude of the normal contact force. In this situation, it is evident that the friction force will be lower than that calculated using Eq. (6.30). Also, since there is no sliding between the crutch tip and the ground, the relative tangential velocity between those contacting surfaces will be zero or very close to zero and, thus, small errors on the estimation of this relative velocity with Eq. (6.23) might lead to significant changes on the direction and magnitude of the calculated friction force.



(a)



(b)



(c)

Figure 6.13 – Comparison of the crutch-ground reaction forces resulting from the sphere-plane contact and experimental data: (a) anteroposterior (x -direction), (b) mediolateral (y -direction) and (c) superoinferior (z -direction) forces on the right crutch.

6.6. Case Study

The purpose of the present section is to integrate all the concepts and methodologies developed and implemented in this work into a final case study. The case study includes the newly formulated kinematic joints and driving constraints, the implemented skeletal muscle modeling procedures, the developed three-dimensional biomechanical multibody model, the experimental data acquired at the Lisbon Biomechanics Laboratory and the associated treatment procedures, the introduction of the assistive device into the model and the interactions that exist between the chosen assistive device and the environment, that is, the model and the ground. The following items are taken into consideration:

- i. the biomechanical multibody model with the simple shoulder is utilized;
- ii. the right and left ankle joint complexes of the model are formulated as modified universal joints;

- iii. the right and left radius and ulna are connected to each other via body-follower joints;
- iv. the point, Euler parameters and the three angle driving constraints are utilized to prescribe the experimental data to the multibody model;
- v. the previously considered muscles (see Table 4.4) are applied to the right lower limb of the model;
- vi. the cost function that minimizes the sum of the cube of the individual average muscle stresses presented in Eq. (4.46) is employed to determine the muscle activations;
- vii. the four-point reciprocal crutch-assisted gait is the chosen pattern to be analyzed;
- viii. the spherical joint is considered as the approach implemented for the crutch-model interaction;
- ix. the sphere-plane contact algorithm is considered to analyze the crutch-ground interaction.

The resulting biomechanical multibody model has a total of 45 degrees-of-freedom, from which three degrees-of-freedom (plantarflexion/dorsiflexion of the right ankle joint complex, inversion/eversion of the right ankle joint complex and flexion/extension of the right metatarsophalangeal joint) are controlled by the muscles and the remaining 42 degrees-of-freedom are controlled by the driving constraints.

The evolution of the right talocrural, talocalcaneal, glenohumeral and radiocarpal joint angles throughout the gait cycle can be consulted in Figure 6.14. It is important to note that the joint angles for the glenohumeral and radiocarpal joints are shown for the sagittal plane only, since it is in this plane that the majority of the joint motion occurs. In addition, the black solid line represents the percentage of gait cycle at which the toe off of the unassisted gait occurs (61% of gait cycle), while the black dashed line denotes the percentage of gait cycle at which the toe off of the crutch-assisted gait occurs (78% of gait cycle). The observation of Figure 6.14a leads to the conclusion that, prior to the toe off, the talocrural joint allows higher plantarflexion in crutch-assisted gait when compared with the unassisted gait. For the talocalcaneal joint, during unassisted gait, prior to the toe off, the joint allows inversion, as opposed to eversion observed in crutch-assisted gait (see Figure 6.14b). During assisted gait, the glenohumeral joint is mainly in a flexed configuration and the magnitude of flexion is higher than that observed for the unassisted gait (see Figure 6.14c). In turn, during crutch-assisted gait, the radiocarpal joint remains in a flexed configuration throughout the entire duration of the gait cycle, while the contrary is true for the unassisted gait (see Figure 6.14d). It can, therefore, be concluded that the use of crutches to help the locomotion of the subject during gait significantly influences the angles of both the lower and upper limb joints. However, it must be noticed that the subject considered in this work is a healthy volunteer with no history of gait disorders that does not depend on the use of crutches for her daily locomotion. Hence, although the obtained results provide some insights into the kinematics of crutch-assisted gait, they may not represent the real cases of disabled patients.

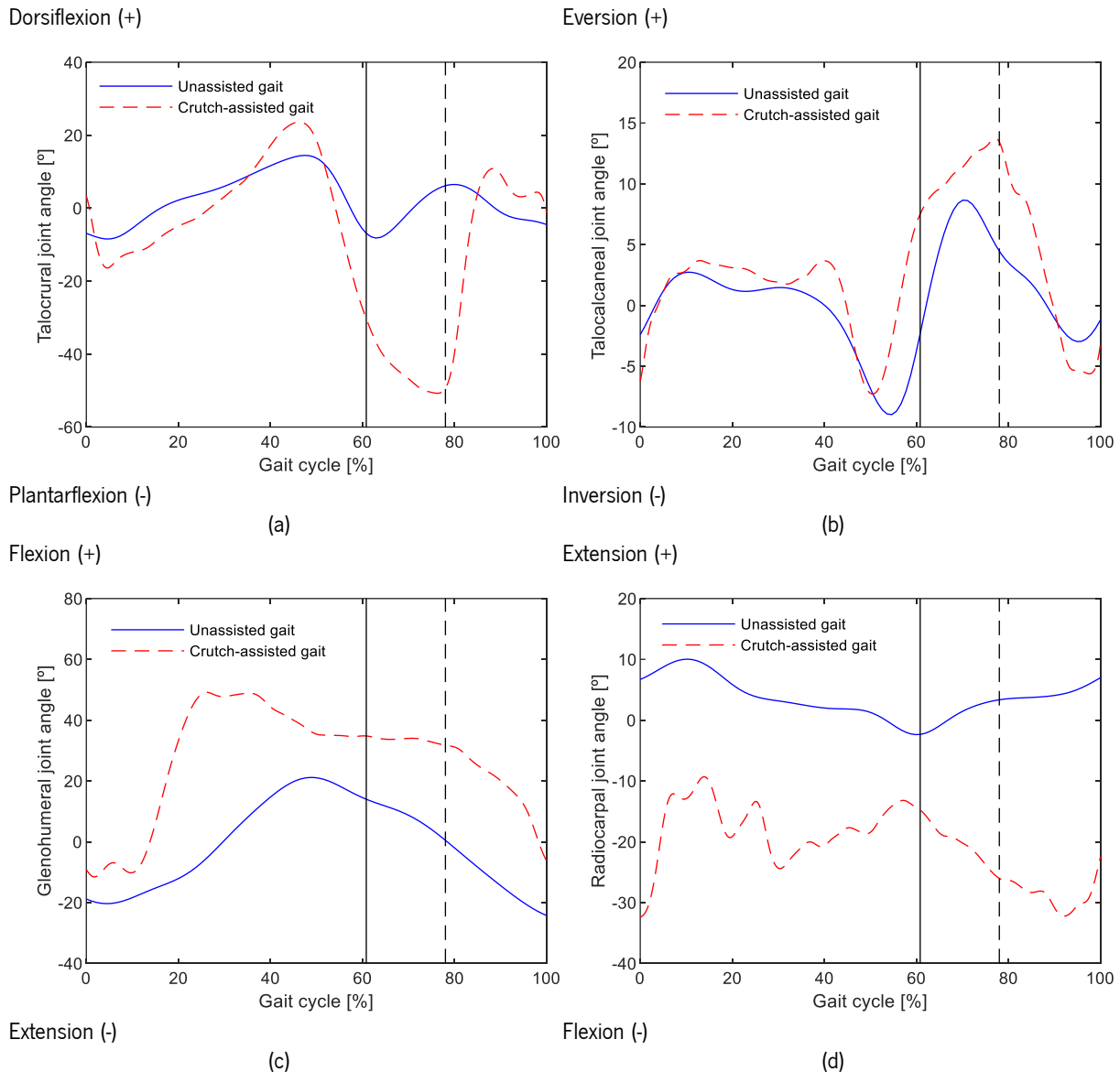


Figure 6.14 – Comparison of the right (a) talocrural, (b) talocalcaneal, (c) glenohumeral and (d) radiocarpal joint angles during unassisted and crutch-assisted gait. The sagittal plane glenohumeral and radiocarpal joint angles are represented. The toe off for the unassisted and assisted gait occurs at 61% (solid line) and 78% (dashed line) of the gait cycle, respectively.

Figure 6.15 shows the reaction forces that develop at the right glenohumeral and radiocarpal joints. It can be observed that, in terms of magnitude, the anteroposterior and mediolateral reaction forces on the glenohumeral joint do not differ significantly when comparing both conditions. In turn, the contrary is true for the radiocarpal joint, in which higher reaction forces are observed in these directions during crutch-assisted gait when compared with unassisted gait. In addition, the superoinferior reaction force for both joints is significantly increased during assisted gait. Besides these conclusions, it is also important to note that, during unassisted gait, none of these joints are subjected to such large reaction forces, as observed in all plots depicted in Figure 6.15. From the analysis conducted in this paragraph, it is, therefore, possible to establish that, during crutch-assisted gait, the radiocarpal joint is, in general, subjected to higher reaction forces than the glenohumeral joint, which suggests that anatomical structures

closer to the assistive device may be more prone to the onset of secondary health conditions. Nevertheless, more analyses with, in a first stage, additional healthy subjects and, later, with disabled patients must be conducted in order to validate these findings.

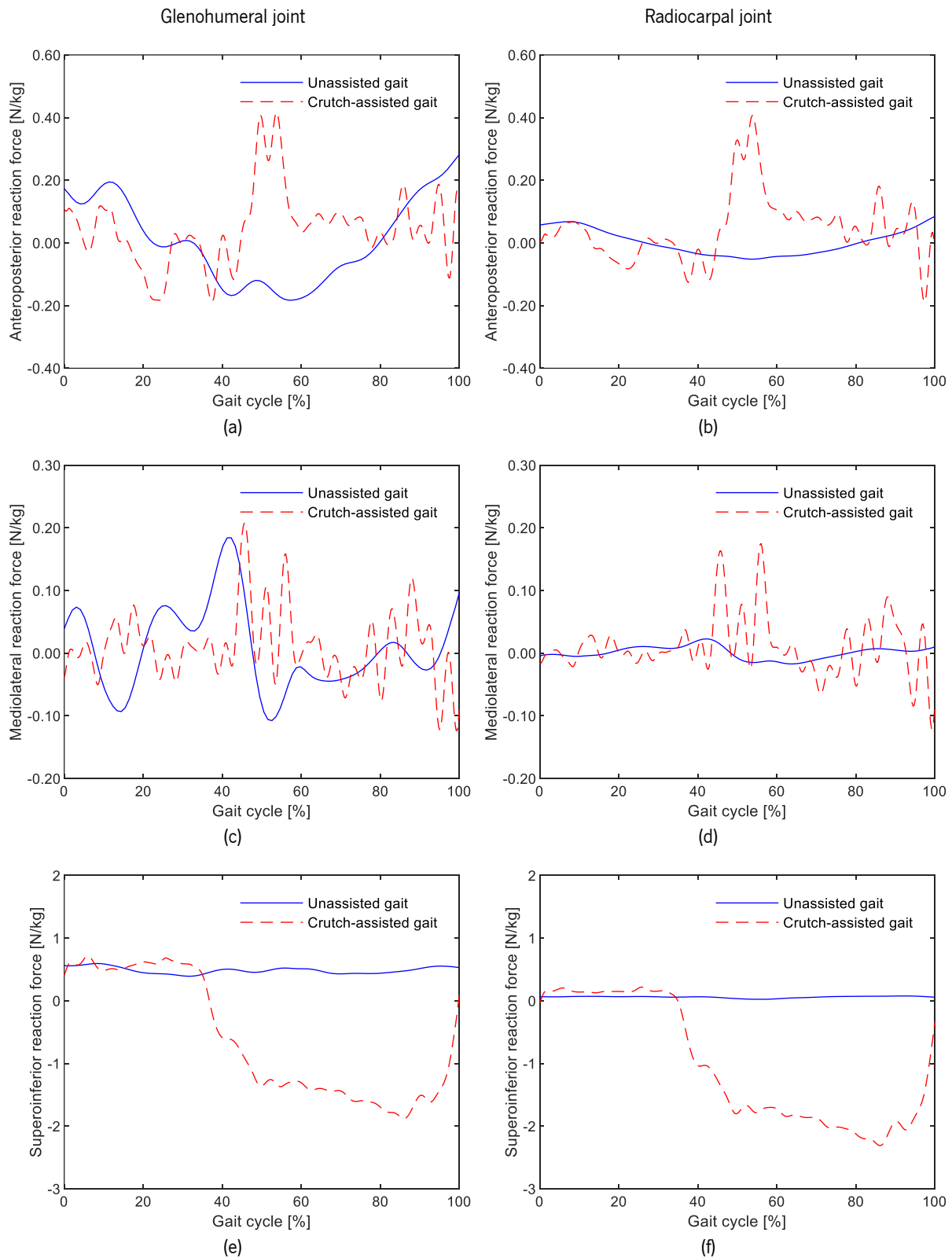
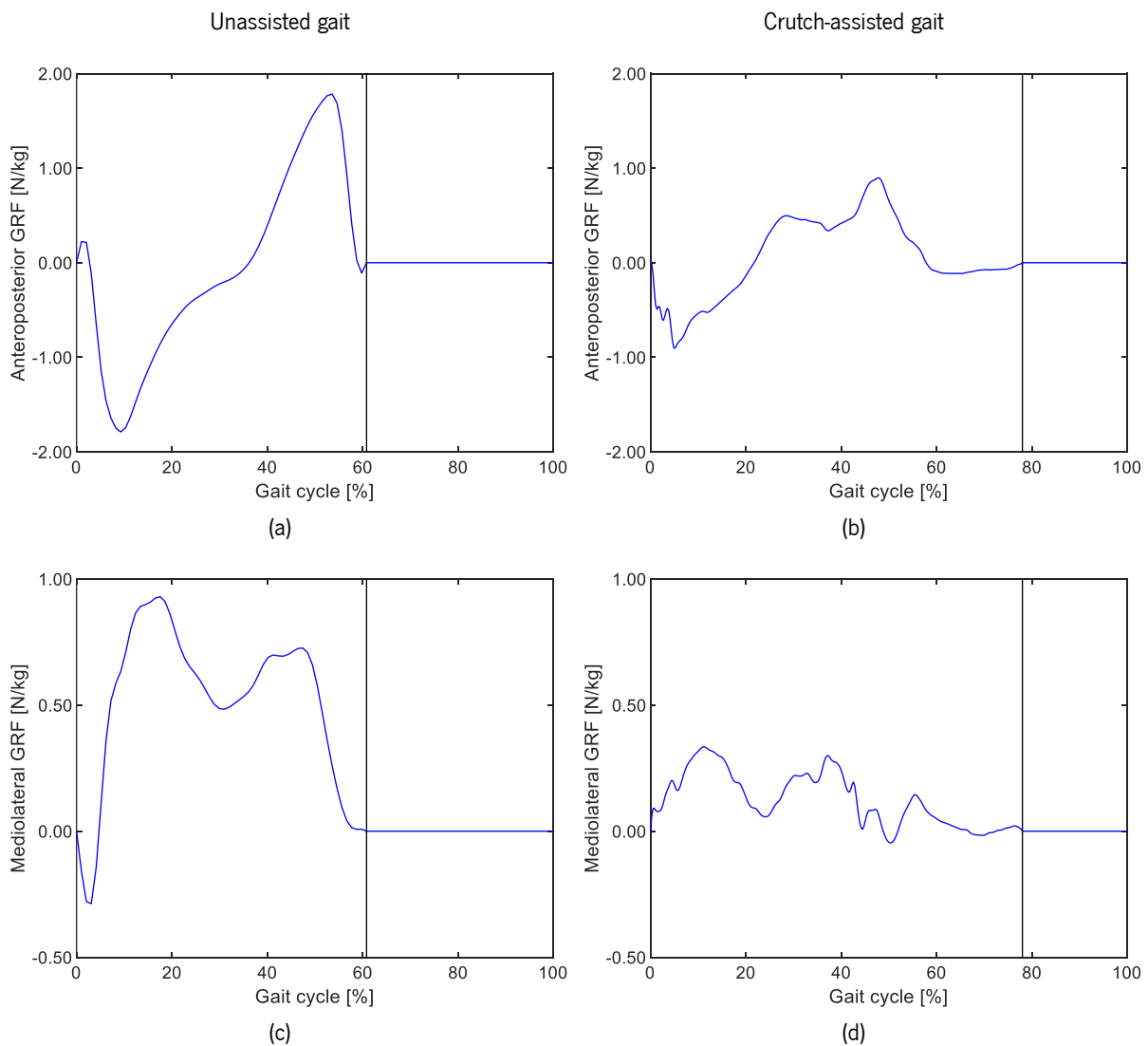


Figure 6.15 – Comparison of the anteroposterior, mediolateral and superoinferior reaction forces developed at the right glenohumeral (a, c, e) and radiocarpal (b, d, f) joints during unassisted and crutch-assisted gait.

The evolution of the reaction forces that develop between the foot and the ground during unassisted and crutch-assisted gait is illustrated in Figure 6.16. It can be seen that, during crutch-assisted gait, the toe off occurs later in the gait cycle (78%) than in unassisted gait (61%). These differences are inherent to the specificities of each gait pattern. An important aspect to take into consideration is the fact that the magnitude of the ground reaction forces (GRF) during crutch-assisted gait is, approximately, half the magnitude observed for the unassisted gait for the anteroposterior and mediolateral directions. For the superoinferior direction the reduction of magnitude is around 30%. This phenomenon might be associated with the fact that, during device-assisted gait, the crutches support a certain quantity of the body weight of the subject, which is the purpose for which they are utilized. However, the body weight that the crutches support is transferred to the upper limbs joints, resulting in higher reaction forces that are not present during unassisted gait, as concluded previously in Figure 6.15 for the glenohumeral and radiocarpal joints. In terms of profile of the plot, the results are similar for the anteroposterior and mediolateral directions, but differ significantly for the superoinferior direction.



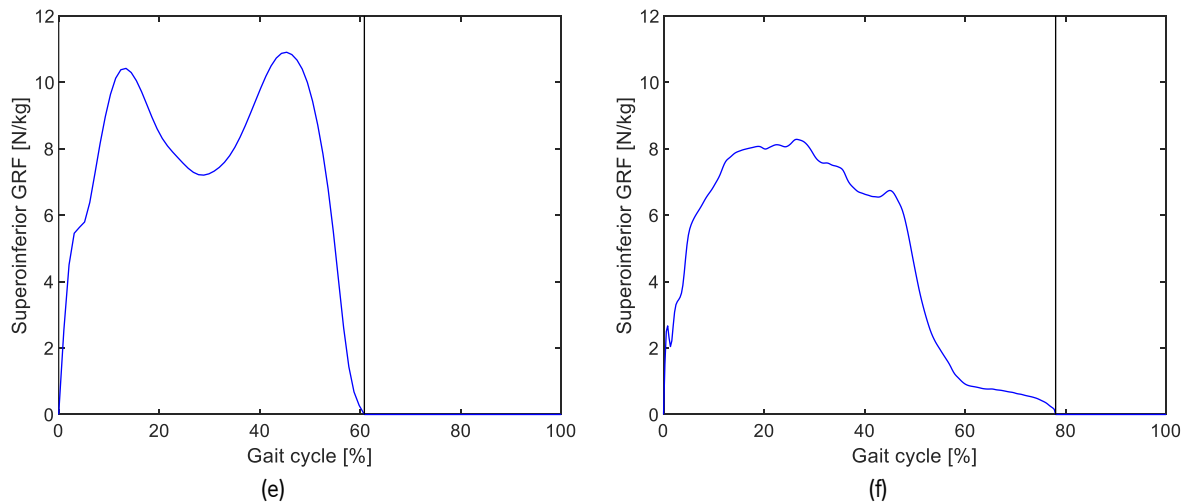
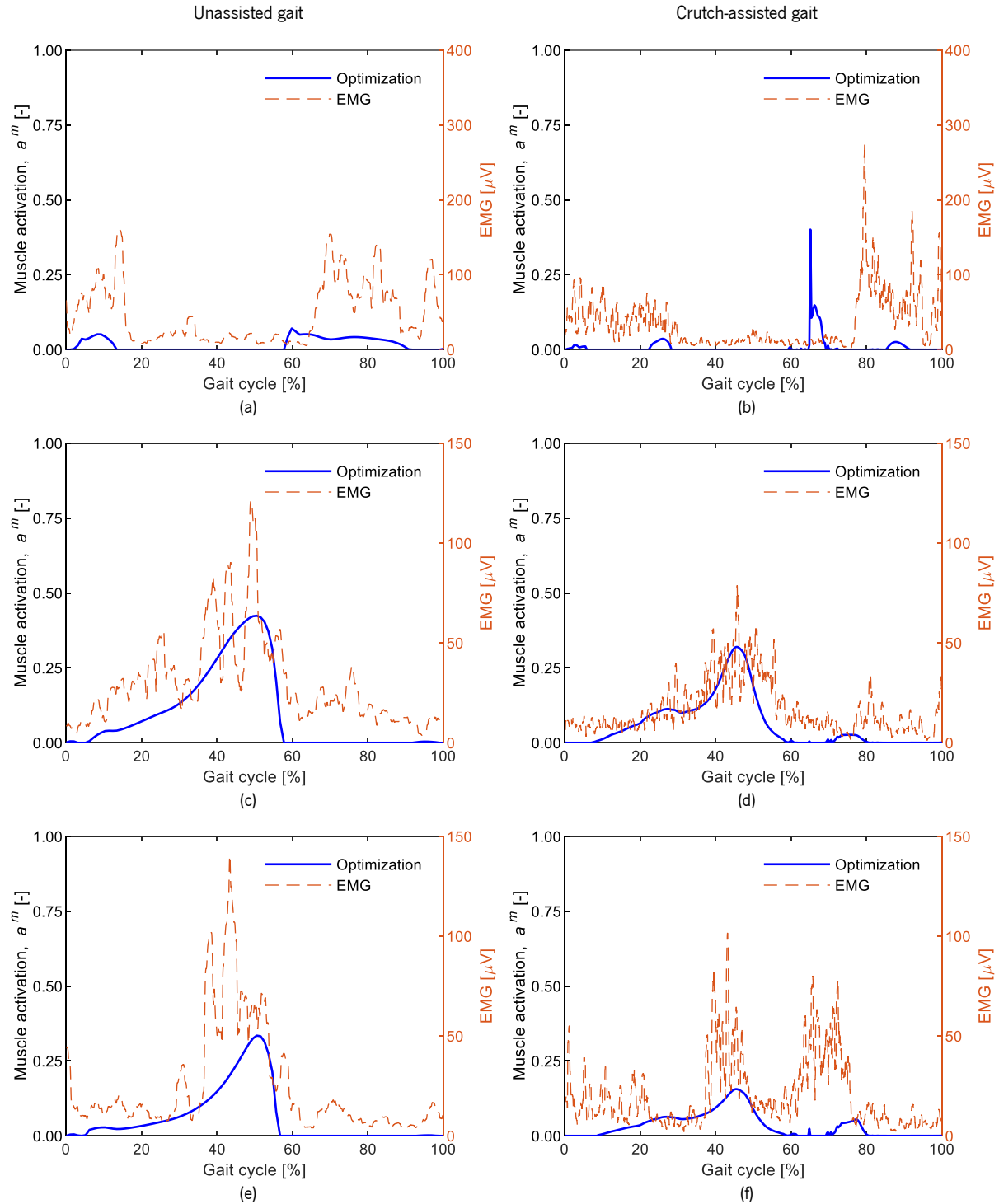


Figure 6.16 – Comparison of the ground reaction forces (GRF) for the right foot during unassisted gait (a, c, e) and crutch-assisted gait (b, d, f). The toe off for unassisted and assisted gait occurs at 61% and 78% of the gait cycle, respectively.

As in the case of unassisted gait, during the experimental data acquisition procedures of crutch-assisted gait carried out at the Lisbon Biomechanics Laboratory, the surface electromyography (sEMG) data of four muscles, namely, the medial and lateral heads of the gastrocnemius, soleus and tibialis anterior, was acquired. However, similarly to the previous experiments, during the treatment of the EMG data it was observed that the activity of the medial head of the gastrocnemius muscle was not correct, and, therefore, the EMG data for this muscle was disregarded. Figure 6.17 presents the muscle activation patterns of the tibialis anterior, soleus, lateral head of the gastrocnemius and peroneus brevis muscles obtained from the optimization and from the sEMG data, and provides a comparison between the unassisted and assisted gait. Concerning the assisted gait, in terms of profile of the plot, the results for the tibialis anterior do not completely agree with the sEMG. According to the sEMG, the muscle should be active from the beginning of the gait cycle until approximately 30% of the gait cycle, and then, from 75% to the end of the analysis. However, although the results provided by the optimization show that the tibialis anterior is active in the beginning of the gait cycle, the activation is not continuous and two small peaks can be observed. The same conclusions can be drawn for the end of the gait cycle since the optimization output indicates two peaks at around 65-70% and 85-92% of the gait cycle, instead of a continuous activation. Concerning the soleus and the lateral gastrocnemius for crutch-assisted gait, the results obtained by the optimization procedure agree well with the sEMG recordings in terms of profile of the plot. It can be observed that, in general, the periods of the gait cycle on which these muscles are active during the optimization match those of the sEMG data, with the exception of the beginning of the gait cycle in which the muscles should be active, but no activation is shown by the optimization. For the peroneus brevis, it can be observed that the optimization procedure indicates that the muscle is active in the beginning and middle of the gait cycle, but these results cannot be confirmed due to the absence of

sEMG recordings and literature data. Generally, the activation for crutch-assisted gait is lower than that obtained for the unassisted gait, with the exception of the tibialis anterior. Finally, it must be mentioned that the optimization procedure did not find a feasible solution for this case study in 20 time steps out of 365 time steps. It is important to recall that this last case incorporates all the methodologies and formulations explained, developed and implemented throughout this work. Therefore, there may be some features that might require further investigation. The scaling procedure applied to the muscle parameters must be validated, as it may be a source of inconsistency that might compromise the obtained results.



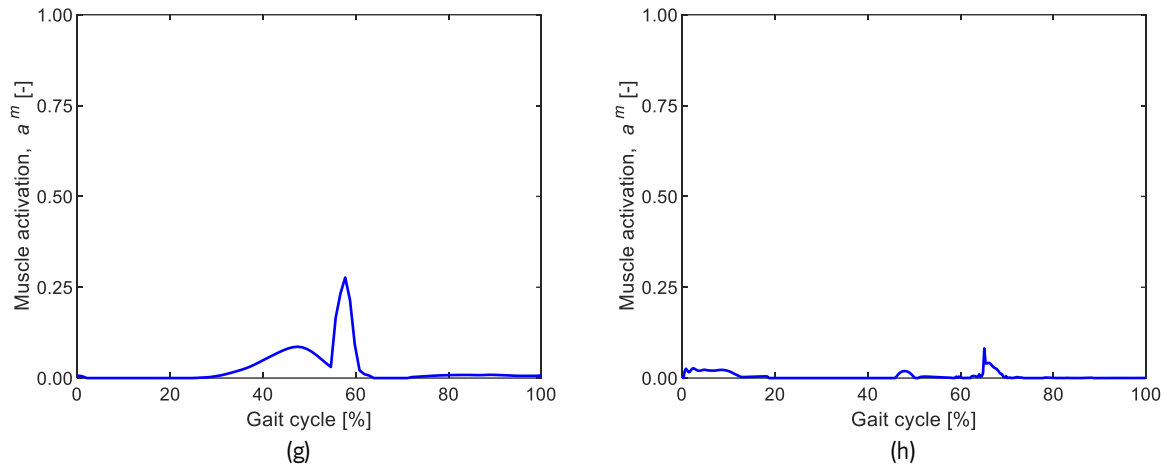


Figure 6.17 – Comparison of the muscle activation patterns for the (a, b) tibialis anterior, (c, d) soleus, (e, f) lateral head of the gastrocnemius and (g, h) peroneus brevis muscles during unassisted and crutch-assisted gait. The toe off for the unassisted and assisted gait occurs at 61% and 78% of the gait cycle, respectively. The optimization results for both conditions are obtained using Eq. (4.46).

6.7. Summary and Discussion

Chapter 6 provides a complete and detailed analysis of device-assisted locomotion. The collaborations established with *Centro de Reabilitação do Norte – Dr. Ferreira Alves* and ORTHOS XXI were crucial for the accomplishment of the objectives of this chapter. As a result from the collaboration with *Centro de Reabilitação do Norte*, an important and useful clinical tool for the analysis and understanding of the pain perceptions of disabled patients was developed. The questionnaire is ready to be applied to patients with any pathological condition and that use any assistive device. In addition, ORTHOS XXI has given important support on the development of the CAD model of the considered C8 closed cuff forearm crutches by providing knowledge on several geometric requirements, as well as on the constituent materials, which ultimately allowed to determine the material properties of this device. Besides unassisted healthy gait, at the Lisbon Biomechanics Laboratory, crutch-assisted gait data was also acquired. The considered gait pattern was four-point reciprocal gait, and two sets of trials were conducted. In the first set, only the feet of the subject contacted the force plates, while no information on the crutch-ground reaction forces was obtained. On the second set of trials, one foot and one crutch contacted the force plate. This procedure was carried out in order to provide an estimate of the profile and magnitude of the normal and tangential crutch-ground reaction forces and to validate the implemented sphere-plane contact algorithm. Two approaches to deal with the interface between the crutch and the biomechanical model were also investigated. The chapter ends with one case study, which integrates and combines all the methodologies developed and implemented in this work. Preliminary findings are reported, which set the foundations for further investigation on device-assisted gait.

“The real test is not whether you avoid this failure, because you won't. It's whether you let it harden or shame you into inaction, or whether you learn from it; whether you choose to persevere.”

Barack Obama

7. CONCLUDING REMARKS

7.1. Conclusions

In this work, the development of an advanced multibody musculoskeletal model of the human movement, accompanied by a comprehensive investigation on device-assisted gait has been presented. Throughout all chapters included in the present document, several novel methodologies and formulations were proposed and discussed, the conclusions of which are highlighted in this section.

Chapter 2 contains a complete and detailed literature review on the topics involved in this work, namely the biomechanical modeling procedures utilized to analyze device-assisted locomotion. The knowledge on this topic served as the foundation for the approaches developed in this doctoral thesis. A rigorous methodology was utilized to find the studies of interest and to conduct the literature reviews. The application of the methodology is demonstrated in the assessment of three main topics of investigation, namely the characteristics utilized in biomechanical models analyzing locomotion assisted by crutches, walkers, wheelchairs and canes, a more in-depth analysis on currently considered crutch modeling procedures, as well as the solutions available in the literature utilized to study the foot-ground interaction problem. Concerning the first topic, it can be concluded that the majority of studies on device-assisted locomotion utilized three-dimensional (3D) models and that unilateral upper extremity models were preferred over full-body or bilateral upper extremity models. In addition, the modeling of the upper extremity was found to be simplified, since few studies included detailed models of the upper limb joints and segments. One of the main conclusions drawn out of the first topic of investigation was that the interest in studying crutch-assisted locomotion has been rising over the years, which laid the foundations for a more in-depth literature review on this topic. Concerning the second reviewed topic, numerous strategies were found for incorporating the crutches into models, but the most commonly utilized strategy was to introduce these devices as independent rigid bodies on the biomechanical model (50% of the studies). In addition, six different approaches to deal with the interface that exists between the crutches

and the model were found. A quarter of the included studies assumed the crutch and other body of the biomechanical model as a unique segment. In this situation, the crutch-model interface does not exist or is implicit. This type of interface was the most common (25% of the studies). Concerning the crutch-ground interface, almost half of the studies instrumented the crutches with forces sensors in order to acquire the reaction forces. It is important to mention that only 4% of the studies utilized contact models. The last reviewed topic was related to the human foot-ground contact models. Points, circles, ellipses, spheres, ellipsoids, rectangular contact elements and surfaces obtained from 3D scanning procedures were found to be the most common types of contact geometries considered. Regarding the resolution of the foot-ground interaction, more than 75% of the studies utilized contact force approaches.

The dynamic analysis of multibody systems has a broad potential of application in biomechanics of motion, as it allows to understand the movement and the dynamic response of the human body in diverse real-world scenarios. All the procedures and methodologies implemented in this work are based on multibody systems methodologies with cartesian coordinates. Hence, in the beginning of Chapter 3 an introduction to the methodologies underlying the dynamic analysis of multibody systems was provided. Afterwards, the formulation of a novel modified universal joint with a massless link was presented, which is specifically developed to accommodate the two particularities of the ankle joint complex of the human foot. All aspects associated with the formulation were explained in detail under the framework of multibody systems methodologies, taking into account the corresponding kinematic constraints, the resulting Jacobian matrix, and the right-hand side of the acceleration constraint equations vector. The performance of the modified universal joint was examined and compared with the solution developed by other authors, which formulated the ankle joint complex as a classical universal joint. Overall, it was concluded that the introduction of the massless link resulted in substantial differences in the mediolateral direction for all variables studied, while the anteroposterior and superoinferior directions presented similar results.

It is known that, in the multibody systems methodology, mechanical joints usually are formulated as classical kinematic constraints such that there is no restriction of the range of motion (RoM) of the joint. Thus, the formulation must include additional restrictions to prevent the joints from performing unacceptable movements and to avoid unrealistic configurations of the connected bodies. Thus, an improved methodology to restrict the range of motion of mechanical joints was also proposed in Chapter 3. Joint resistance moments are applied to the bodies connected by the joint to mimic the dissipative behavior of the materials constituent of joints and to prevent unacceptable configurations of those bodies. The methodology was investigated in the dynamic modeling and simulation of one demonstrative example of application, namely a three-dimensional biomechanical model of the human leg, main foot and toes.

For the application of the RoM methodology, the modified universal joint can be thought of as two revolute joints, which means that the RoM associated with each joint axis must be restricted independently and two different circumduction cones must be constructed. Due to the fact that, in a modified universal joint, there is a massless link connecting the two bodies, the joint motion-restricting moment is directly applied to the reference body and to the massless link. Thus, a process of force and moment transfer from the massless link to both the moving and reference bodies was considered, and it was explained in detail in this work. From the obtained results, it could be concluded that the proposed methodology correctly restricted the RoM of the ankle joint complex of the human foot and it has potential of being further applied to the dynamic simulation of other biomechanical multibody models.

In Chapter 3, the formulation of five different types of driving constraints was also explained in detail. The driving constraints are expressed as functions of the time variable and are typically obtained experimentally by using an optoelectronic motion capture system. The driving constraints were specifically formulated to drive the degrees-of-freedom of the considered biomechanical model and allowed to guide a generic point G , an arbitrary Euler parameter, the angle between two vectors $\mathbf{a}_i$ and $\mathbf{b}_j$, the angle between a vector $\mathbf{a}_i$ and a massless link vector $\mathbf{d}$, and the angle between a vector $\mathbf{a}_i$ and a vector projected on a plane $\mathbf{b}_{j,p}$. The performance of the developed formulations was verified at the end of the chapter through the analysis of an application example. From the results, it was concluded that the driving constraints allowed to correctly guide the degrees-of-freedom of the biomechanical multibody model analyzed in the example. In addition, the violation of the constraint equations at the position and velocity levels was also evaluated, which magnitude was considered to be negligible. These results indicate that all constraints of the biomechanical model, including joint and driving constraints, were not violated throughout the analysis, which further validates the proposed driving constraint formulation.

In Chapter 4, all concepts associated with skeletal muscle modeling were specified. An explanation of the anatomical and physiological characteristics of the human skeletal muscle was provided at the beginning of the chapter. There are several events occurring from neural signal generation until the production of muscular force, namely the muscular stimulation, the muscular activation and the muscular contraction. In this work, the muscle contraction dynamics was approached, which corresponds to the process of transforming the muscle activation into muscle force. The muscle model utilized in the present document to reproduce the contraction dynamics is a variant of the Hill model and it is composed of an active contractile element arranged in parallel with an elastic element. Also, skeletal muscles were spatially defined by the coordinates of a series of points connected by line segments, and were introduced into the multibody model as external forces. An important aspect to take into consideration is that, since

the number of muscle activations exceeds the number of degrees-of-freedom of the biomechanical models, a unique solution for the analytical determination of the muscle forces cannot be obtained. Thus, the solution for this problem can be found through the use of an optimization procedure, which allows to estimate the optimal muscle activations according with the minimization of cost functions that simulate the decisions taken by the central nervous system when executing a certain task. Two examples of application were analyzed. The results obtained for the simple example, a double pendulum multibody model, allowed to conclude that the implemented methodology is correctly working and producing expected results. The aim of the second example of application was to demonstrate the consideration of muscles into ankle joint complex of the human foot. The results were physiologically sound for the muscle activations, muscle moment arms and joint moments. The magnitude and profile of the plots for the talocrural and talocalcaneal joint moments were in accordance with the literature for healthy human gait. However, the joint moment resulting from the sum of the moments of all muscles acting around each joint did not completely coincide with the joint moment obtained from the joint drivers of the same model without muscles. Thus, further analysis should be performed to understand and improve the results.

The development of two advanced biomechanical models of the human movement was achieved in Chapter 5. The first model considered the glenohumeral joint as the only joint that connects the upper part of the trunk to the arm. The second model utilized a more detailed modeling of the shoulder joint complex, including the glenohumeral, sternoclavicular, acromioclavicular and scapulothoracic joints. In addition, a new type of kinematic joint has been proposed in Chapter 5 to connect the radius and the ulna. The new joint is termed body-follower joint and allows to constrain the translational and orientational coordinates of a body j relative to the translational and orientational coordinates of a body i , therefore removing the six degrees-of-freedom associated with body j . All the acquisition and treatment processes of the experimental data at the Lisbon Biomechanics Laboratory have been approached and described, including the adopted kinematic consistency procedure. Kinematic, kinetic and surface electromyographic (sEMG) data were recorded. The chapter ends with one example that is utilized to demonstrate the application of the data acquired at the laboratory to the biomechanical multibody model.

A detailed analysis of device-assisted gait, with a particular focus on crutches, was provided in Chapter 6. The collaborations established with *Centro de Reabilitação do Norte – Dr. Ferreira Alves* and ORTHOS XXI were crucial for the accomplishment of the objectives of this chapter. As a result from the collaboration with Centro de Reabilitação do Norte, a useful clinical tool for the analysis of the pain perceptions of disabled patients was developed. In addition, ORTHOS XXI has given significant support on the development of the CAD model of the considered C8 closed cuff forearm crutches. The cooperation

and combined expertise of *Centro de Reabilitação do Norte*, which communication was established with medical doctors specialized in spinal cord injury, and ORTHOS XXI, a leading medical devices manufacturer, were a strong asset for this doctoral work. Their firsthand insights into the clinical aspects of spinal cord injury rehabilitation and practical experience with medical device design brought a crucial perspective to the work. By bridging the gap between academia, industrial and clinical practice, these collaborators ensured the alignment with real-world applications and the specific needs of patients.

In this work, the crutches were introduced into the model using two approaches. First, a fixed joint was considered between the hand and the crutch, which was then substituted by a spherical joint. The results obtained with the spherical joint approach were closer to the experimental data acquired at the laboratory, and, therefore, this was the approach chosen for further studies on device-assisted gait. Concerning the interface between the crutch and the ground, the sphere-plane contact detection algorithm was utilized, in which the crutch tip was assumed to be a sphere and the ground was considered a plane. The profile of the obtained penetration was in accordance with the periods of the contact between each crutch and the ground for the four-point reciprocal gait under analysis. It is also important to mention that the obtained magnitude for the penetration was within acceptable values concerning the sensitivity of the infrared cameras utilized at the Lisbon Biomechanics Laboratory. Concerning the crutch-ground reaction forces resulting from the sphere-plane contact algorithm, the results obtained for the anteroposterior and mediolateral forces must be improved, but the normal contact force showed good agreement with the experimental data. A final case study which integrated the approaches developed in this work was explained at the end of Chapter 6. Overall, the obtained preliminary findings were good and set the foundations for further investigation on device-assisted gait.

7.2. Future Developments

In the present work, important aspects that allowed the study of crutch-assisted gait were approached. First, a detailed literature review on biomechanical models utilized for the analysis of device-assisted locomotion was provided, with particular emphasis on the modeling procedures of crutches. A three-dimensional biomechanical multibody model of the human movement was developed, which included the formulation of kinematic joints specific to the model, namely the modified universal and the body-follower joints. In addition, several driving constraints were developed and implemented in order to guide all the degrees-of-freedom of the model using the experimental data acquired at the Lisbon Biomechanics Laboratory. All processes associated with the data acquisition and treatment were approached. The explanation of the concepts related to skeletal muscle modeling and the implementation

of all the associated procedures, namely the muscle contraction dynamics, the introduction of muscles into the equations of motion and the optimization, was provided in detail. Finally, specific concepts on crutch-assisted gait were investigated. For this purpose, important collaborations with *Centro de Reabilitação do Norte – Dr. Ferreira Alves* and ORTHOS XXI were established. The detailed analysis of the interfaces that exist between the considered assistive device and the model or the ground was conducted. While the approaches presented and developed throughout this document represent advances in the state-of-the-art, future developments are required in order to address some limitations associated with this work. Therefore, in the following paragraphs some recommendations for future studies are provided.

Besides the concepts mentioned in the above paragraph, in this work, a novel methodology to restrict the range of motion of mechanical joints has been proposed. The restriction of the range of motion of joints is of particular interest in optimization studies considering a forward dynamics analysis, as it ensures that the simulation does not converge into unrealistic solutions. The reliability of a dynamic simulation of a multibody system is highly dependent on the accuracy of its mechanical response. Therefore, the development of methodologies that realistically and accurately restrict the range of motion of mechanical joints is of paramount importance in order to correctly model multibody systems, providing more accurate results. In this work, the methodology to restrict the range of motion of joints was applied to a complex case of the biomechanics of motion discipline. In future studies, the proposed methodology can be extended for application in other areas of investigation, including robotics and crashworthiness.

Additionally, a complete literature review on the available methodologies usually utilized to study the interaction between the foot and the ground in the human locomotion has been presented. In this work, the foot-ground contact problem was approached by the experimental acquisition of the ground reaction forces (GRF) using three force plates existing at the Lisbon Biomechanics Laboratory. The recorded data was directly introduced into the biomechanical multibody model in the vector of external generalized forces, $\mathbf{g}$. However, the measurement and data acquisition of the GRF are constrained in the number of human steps, since the experimental apparatus and platforms have limited lengths. With the purpose of overcoming this drawback, several formulations to mimic the human foot-ground interaction have been proposed in the literature, which provide numerical approaches to calculate the GRF without the need of any experimental measurement. Hence, future developments associated with this work should aim at implementing the foot-ground interaction formulations provided in the literature review of this document. However, it is important to note that it is still a quite challenging problem to accurately represent the contact mechanics when the geometric and material properties are of complex natures, such as in the case of the human foot-ground interface.

Concerning the skeletal muscle modeling procedures, some aspects should be further developed and investigated. In this work, a linear scaling procedure was taken into consideration in order to determine the muscle parameters that fitted the subject under analysis. This type of scaling may be a source of errors and inconsistencies, since the scaling relation may not be linear and the estimated parameters may not be close to the real values for the subject, particularly the locations of the origin, insertion and via-points, which may compromise the capacity of the muscle to generate force and produce a certain movement. In addition, the pennation angle and the maximum isometric muscle force were not scaled. Hence, more robust and advanced methods to deal with the scaling of the muscle parameters should be investigated. Another important aspect that should be considered in future studies is the implementation of methodologies that consider the wrap of muscles around anatomical structures, such as the obstacle-set method for representing muscle paths proposed by Garner & Pandy (2000). The accurate estimation of the muscles forces and joint moments is dependent on the correct definition of the muscle path and direction of the muscle force. Typically, some muscles of the human body are forced to wrap around the anatomical structures, such as bones and neighboring tissues, and, thus, the straight-line model with via-points utilized in this work might not adequately represent those situations, which may compromise the obtained results. In addition to these aspects, only eleven muscles were considered in this work. Future studies should aim at introducing more muscles into the biomechanical multibody model, specifically those associated with the upper extremity, such as the biceps brachii or the trapezius muscles, since they are relevant for the analysis of device-assisted locomotion. Finally, two other aspects could be objective of further investigation, namely the analysis of other optimization criteria, such as the min/max criterion proposed by Rasmussen et al. (2001), and the consideration of muscle fatigue.

The three-dimensional biomechanical multibody models developed in this work assume that there is no relative movement between the radius and the ulna, since a body-follower joint is utilized to connect the two rigid bodies via the radioulnar joint. This procedure was adopted in order to facilitate the acquisition of the experimental data and the application of the driving constraints to the model. Although this approach precludes the pronation and supination movements of the forearm, they are considered at the humeroulnar joint, which is formulated as a universal joint that allows flexion/extension of the arm and pronation/supination of the forearm. However, in order to increase the biofidelity of the multibody model, one option would be to implement the approach proposed by Kecskeméthy & Weinberg (2005). In addition, for a more detailed analysis of the dynamics of the shoulder joint complex during device-assisted gait, the biomechanical model with the detailed shoulder should be utilized. To this end, a novel marker set protocol specific to this model and to the additional rigid bodies considered at the

shoulder must be developed. The detailed model may be capable of providing better insights into the reaction forces that are transmitted from the assistive device to the glenohumeral, sternoclavicular, acromioclavicular and scapulothoracic joints. Finally, the proposed kinematic consistency procedure could be improved. The purpose would be to, besides obtaining kinematically consistent position and velocities via the direct correction approach, implement an optimization approach. The objective would be to minimize the error between the location of the joints calculated as the midpoint between the experimental markers and the location of the joints defined in the model. The implementation of the improved kinematic consistency procedure could lead to more accurate results.

Concerning the analyses performed with device-assisted gait, some future developments can also be carried out. In this work, only four-point crutch-assisted gait was considered. In future studies, other gait patterns, namely the two-point reciprocal gait or the swing-through gait, and other movements, such as climbing stairs and sitting, could be investigated. As previously stated, when referring to the foot-ground contact, in mechanical systems with complex geometries, accurately modeling the interaction between surfaces is a crucial aspect for predicting their dynamic behavior, especially in systems where the contact phenomena plays a significant role. The same logic can be applied to the crutch-ground interaction. In this work, the sphere-plane contact algorithm was implemented to model the contact between the crutch and the ground. The drawbacks associated with the sphere-plane contact include the fact that only one point of contact between the two surfaces is considered and the geometry of the crutch tip is not accurately represented. One class of geometric surfaces that frequently arises in practical applications are toroidal surfaces, which can be utilized to represent several elements, such as tires, seals, and various types of rings. In future studies, toroidal surfaces could be utilized to represent the crutch tip, thus improving the geometric similarity. However, the torus, with its continuous circular symmetry, presents a unique challenge in contact mechanics due to its nontrivial geometry, which often results in complex contact interactions when dealing with planar surfaces or other curved bodies. Another aspect to improve the results obtained for the contact forces could be to utilize co-simulation approaches, by considering multibody dynamics methodologies and finite element methods (FEM). Crutch instrumentation procedures could also be carried out in order to record the crutch-ground reaction forces simultaneously with the acquisition of the GRF with the force plates and motion data. Finally, other assistive devices can be object of further investigation, including walkers and wheelchairs.

“The more I read, the more I acquire, the more certain I am that I know nothing.”

Voltaire

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LIST OF PUBLICATIONS

Papers in Scientific Journals

1. **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., An integrated approach for the experimental and computational analysis of crutch-assisted gait. *In preparation*.
2. **Silva, M. R.**, Gonçalves, S. B., Marques, F., Flores, P. and Silva, M. T., Validation of muscle models in multibody dynamics: a collaborative collection of benchmark cases. *In preparation*.
3. Sousa, M. F., **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., A review on crutch-assisted modeling with focus on the interactions with the ground and with the human body. *In preparation*.
4. Rodrigues, F., **Silva, M. R.**, Silva, F. S., Madeira, S., Carvalho, Ó., Electric Current Application on Dental Implant Biofilms: Review. *Journal of Functional Biomaterials*, vol. 15, pp. 197. <https://doi.org/10.3390/jfb15070197>, 2024
5. **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., A methodology to restrict the range of motion of joints: Application to the ankle joint complex. *Mechanism and Machine Theory*, vol. 198, pp. 105654, 2024.
6. **Silva, M. R.**, Coelho, J., Gonçalves, F., Novais, F. and Flores, P., Multibody Dynamics in Robotics with Focus on Contact Events. *Robotica*, 2024.
7. **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., An improved methodology to restrict the range of motion of mechanical joints. *Nonlinear Dynamics*, vol. 112(6), pp. 4227–4256, 2024.
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11. Saraiva, L., **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., A review on foot-ground contact modeling strategies for human motion analysis. *Mechanism and Machine Theory*, vol.177 pp. 105046, 2022.
12. Roupa, I., **Silva, M. R.**, Marques, F., Gonçalves, S. B., Flores, P. and Silva, M. T., On the modeling of biomechanical systems for human movement analysis – a narrative review, *Archives of Computational Methods in Engineering*, vol. 29(7), pp. 4915–4958, 2022.
13. Marques, A. C., Cunha, Â., **Silva, M. R.**, Osendi, M. I., Silva, F. S., Carvalho, Ó. and Bartolomeu, F., Inconel 718 produced by Laser Powder Bed Fusion: an overview of the influence of processing parameters on Microstructural and Mechanical properties. *International Journal of Advanced Manufacturing Technology*, vol. 121(9-10), pp. 5651–5675, 2022.
14. Cunha, Â., Marques, A. C., **Silva, M. R.**, Bartolomeu, F., Silva, F. S., Gasik, M., Trindade, B. and Carvalho, Ó., Laser powder bed fusion of the steels used in the plastic injection mould industry: a review of the influence of processing parameters on the final properties. *International Journal of Advanced Manufacturing Technology*, vol. 121(7-8), pp. 4255–4287, 2022.
15. **Silva, M. R.**, Andrade, R., Cardoso, F. S., Oliveira, S., Catarino, S. O., Carvalho, Ó., Silva, F. S., Espregueira-Mendes, J., and Flores, P., Light stimulation on tenocytes: A systematic review of in vitro studies. *Porto Biomedical Journal*, vol. 7(4), pp. e176, 2022.
16. **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., A compendium of contact force models inspired by Hunt and Crossley's cornerstone work. *Mechanism and Machine Theory*, vol. 167, pp. 104501, 2022.

17. Dantas, T., Padrão, J., **Silva, M. R.**, Pinto, P., Madeira, S., Vaz, P. and Silva, F. S., Bacteria co-culture adhesion on different texturized zirconia surfaces, *Journal of the Mechanical Behavior of Biomedical Materials*, vol. 123, pp. 104786, 2021.
18. **Silva, M. R.**, Freitas, B., Andrade, R., Carvalho, Ó., Renjewski, D., Flores, P., Espregueira-Mendes, J., Current perspectives on the biomechanical modelling of the human lower limb: a systematic review. *Archives of Computational Methods in Engineering*, vol. 28(2), pp. 601–636, 2021.
19. **Silva, M. R.**, Freitas, B., Andrade, R., Espregueira-Mendes, J., Silva, F. S., Carvalho, Ó., and Flores, P., Computational modelling of the bioheat transfer process in human skin subjected to direct heating and/or cooling sources: a systematic review. *Annals of Biomedical Engineering*, vol. 48(6), pp. 1616–1639, 2020.

Books

1. Flores, P., Marques, F. & **Silva, M. R.** (2024). MMT Symposium – Mechanism and Machine Theory Symposium, Book of Abstracts. ISBN: 978-989-33-6448-2
2. Flores, P., Marques, F., **Silva, M. R.**, & Novais, F. (2023). Projeto Integrador em Engenharia Mecânica. Quântica Editora. doi: 10.61875/9789899177215
3. Marques, F., Quental, C., Flores, P. & **Silva, M. R.** (2022). 2nd Portuguese Conference on Multibody System Dynamics, Book of Abstracts. ISBN: 978-989-33-4087-5

Book Chapters

1. **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., Modelling Spherical Joints in Multibody Systems, In: Pucheta, M., Cardona, A., Preidikman, S., Hecker, R. (eds) Multibody Mechatronic Systems. MuSMe 2021. *Mechanisms and Machine Science*, vol. 110. Springer, Cham, 2022.

2. Cunha, Â., Marques, A. C., Monteiro, F., Silva, J. A., **Silva, M. R.**, Trindade, B., Ferreira, R., Flores, P., Carvalho, Ó, Silva, F. S., Braga, A. C., Tribological Behavior of 316L Stainless Steel Reinforced with CuCoBe + Diamond Composites by Laser Sintering and Hot Pressing: A Comparative Statistical Study. In: Gervasi, O., et al. *Computational Science and Its Applications – ICCSA 2020. ICCSA 2020. Lecture Notes in Computer Science*, vol. 12251. Springer, Cham., 2020.

National and International Conferences

1. **Silva, M. R.**, Marques, F., Gonçalves, S. B., Tavares da Silva, M., Flores, P., Computational and Experimental Study of the Interaction Between a Crutch and a Biomechanical Human Model. *11^o Congresso Nacional de Biomecânica (CNB 2025)*, Sesimbra, Portugal, February 21-22, 2025.
2. **Silva, M. R.**, Marques, F., Gonçalves, S. B., Tavares da Silva, M., Flores, P., Modeling and Analysis of the Interaction Between the Crutch and the Ground in Human Locomotion. *11^o Congresso Nacional de Biomecânica (CNB 2025)*, Sesimbra, Portugal, February 21-22, 2025.
3. **Silva, M. R.**, Marques, F., Gonçalves, S. B., Tavares da Silva, M., Flores, P., Computational and Experimental Analysis of Crutch-Assisted Gait: Findings from a Case Study. *IFTToMM Young Faculty Group Symposium on Emerging Fields in Mechanism and Machine Science (IFTToMM YFG-MMS)*, online, November 19-21, 2024.
4. Marques, F., **Silva, M. R.**, Contact modeling between torus surfaces and plane using compliant force models. *IFTToMM Young Faculty Group Symposium on Emerging Fields in Mechanism and Machine Science (IFTToMM YFG-MMS)*, online, November 19-21, 2024.
5. Sousa, M. F., **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., On the modeling of crutch-assisted locomotion: examining the interfaces with the ground and with the human body, *MMT Symposium – Mechanism and Machine Theory Symposium*, Guimarães, Portugal, June 26-28, 2024.

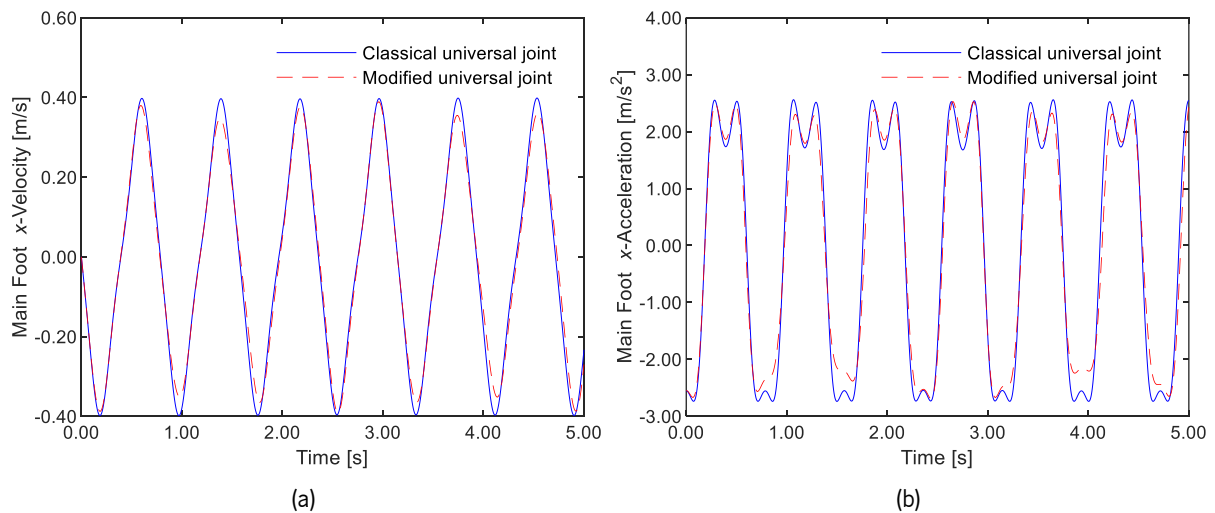
6. Novais, F., **Silva, M. R.**, Gomes, I., Puga, H. and Flores, P., A simple and comprehensive approach to formulate and solve dynamics problems in a non-traditional engineering course, *MMT Symposium – Mechanism and Machine Theory Symposium*, Guimarães, Portugal, June 26-28, 2024.
7. Sousa, M. F., **Silva, M. R.**, Marques, F., Gonçalves, S. B., Silva, M. T. and Flores, P., Experimental and computational analysis of the human gait with crutches, *MMT Symposium – Mechanism and Machine Theory Symposium*, Guimarães, Portugal, June 26-28, 2024.
8. **Silva, M. R.**, Sousa, M. F., Marques, F., Gonçalves, S. B., Silva, M. T. and Flores, P., Modeling and analysis of the ankle joint complex with muscles, *MMT Symposium – Mechanism and Machine Theory Symposium*, Guimarães, Portugal, June 26-28, 2024.
9. **Silva, M. R.**, Marques, F., Gonçalves, S. B., Silva, M. T. and Flores, P., Modeling the ankle articular complex: a computational and experimental analysis, *ECCOMAS Thematic Conference on Multibody Dynamics*, Lisboa, Portugal, July 24-28, 2023.
10. Saraiva, L., **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., Current perspectives on the modeling of the foot-ground interaction for human motion analysis, *2ª Conferência Nacional de Dinâmica de Sistemas Multicorpo (DSM2022)*, Guimarães, Portugal, December 5-6, 2022.
11. Saraiva, L., **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., A foot-ground contact model for human motion analysis, *2ª Conferência Nacional de Dinâmica de Sistemas Multicorpo (DSM2022)*, Guimarães, Portugal, December 5-6, 2022.
12. **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., Current evidence on biomechanical modeling for the analysis of crutch-assisted gait, *2ª Conferência Nacional de Dinâmica de Sistemas Multicorpo (DSM2022)*, Guimarães, Portugal, December 5-6, 2022.
13. **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., A novel methodology to restrict the range of motion of human articulations, *2ª Conferência Nacional de Dinâmica de Sistemas Multicorpo (DSM2022)*, Guimarães, Portugal, December 5-6, 2022.

14. **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., A New Model to Study the Talocrural-Talocalcaneal Articular Complex of the Human Foot., *IX International Conference on Computational Bioengineering (ICCB 2022)*, Lisboa, Portugal, December 5-6, 2022.
15. **Silva, M. R.**, Marques, F., Silva, M. T. and Flores, P., Modelling Spherical Joints in Multibody Systems., *7th International Symposium on Multibody Systems and Mechatronics (MuSME 2021)*, Córdoba, Argentina, online, October 12-15, 2021.
16. Cunha, Â., Marques, A. C., Monteiro, F., Silva, J. A., **Silva, M. R.**, Trindade, B., Ferreira, R., Flores, P., Carvalho, Ó, Silva, F. S., Braga, A. C., Tribological Behavior of 316L Stainless Steel Reinforced with CuCoBe + Diamond Composites by Laser Sintering and Hot Pressing: A Comparative Statistical Study. *Computational Science and Its Applications – ICCSA 2020. ICCSA 2020. Lecture Notes in Computer Science*, Cagliari, Italy, online, July 1-4, 2020.

Appendix A – Time evolution of the velocity and acceleration of the center of mass of the main foot and phase portrait plots

The results presented in this appendix are related to the analysis carried out in the application example analyzed in section 3.5.1, in which two kinematic joint models for the ankle joint complex of the human foot are compared and discussed.

The plots of Figure A.1 depict time evolution of the velocity and acceleration of the center of mass of the main foot of the biomechanical multibody model. The most important differences between both kinematic joint models tested for the ankle joint complex are observed in the mediolateral direction (see Figure A.1c and Figure A.1d). The plots differ in magnitude, in which the modified universal joint allows higher velocity and acceleration magnitudes of the center of mass of the main foot, and they are inverted, meaning that when a positive velocity/acceleration value is observed in one joint model, the other model presents a negative value, and vice-versa. This phenomenon is associated with the talocalcaneal joint location, which is influenced by the consideration or not of the massless link. Concerning the anteroposterior (Figure A.1a and Figure A.1b) and superoinferior (Figure A.1e and Figure A.1f) directions, the results are quite similar. Small differences can be visible in the peaks for the velocity and acceleration, with the classical universal joint exhibiting slightly higher magnitude values.



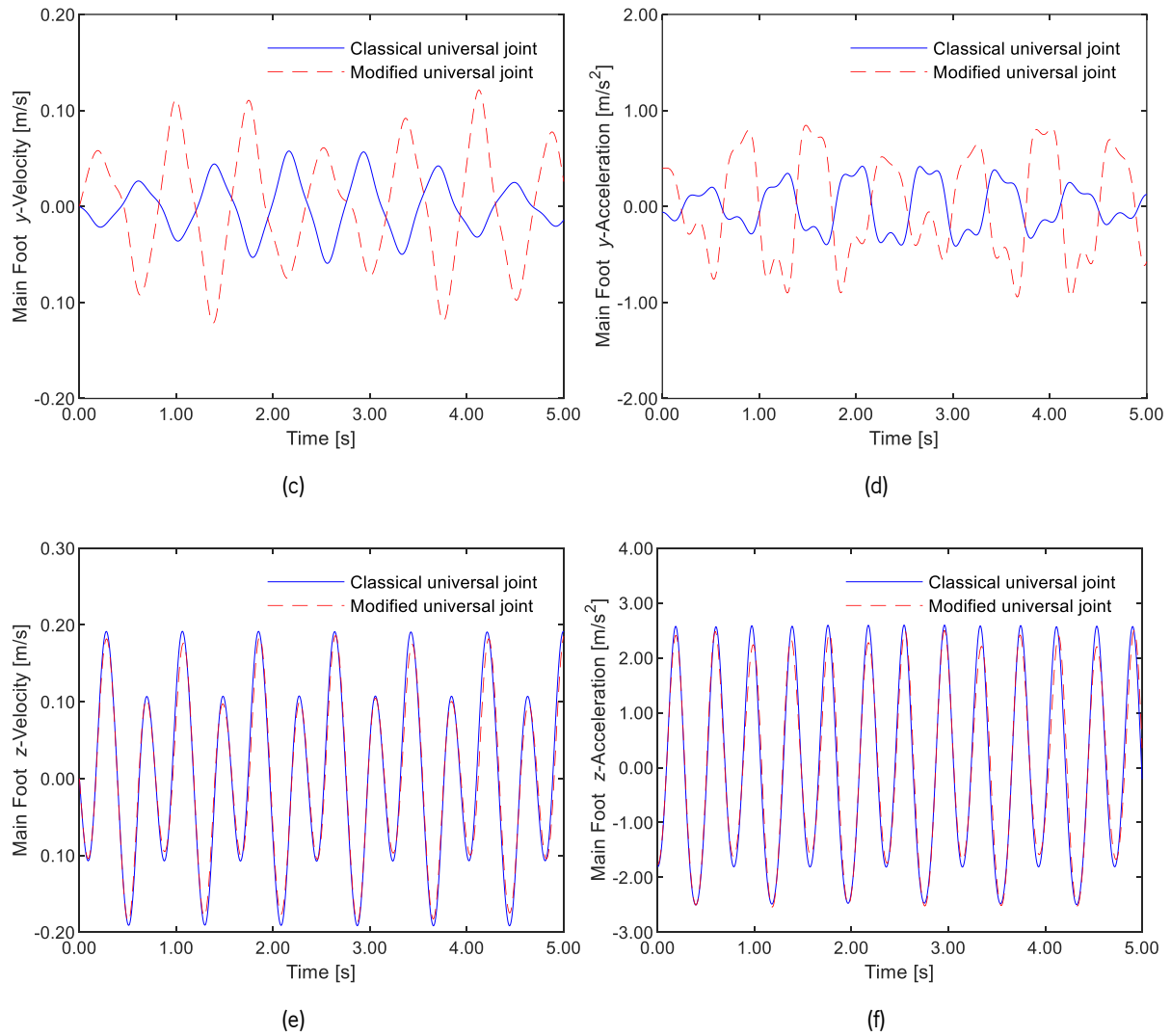


Figure A.1 – Influence of the joint model considered for the ankle joint complex of the human foot on the response of the biomechanical model. Velocity (a), (c), (e), and acceleration (b), (d), (f) of the center of mass of the main foot segment.

Figure A.2 shows the phase portraits of the two joint models tested for the ankle joint in section 3.5.1. The plots include the x -component, the y -component and the z -component of the position of the center of mass of the main foot versus its velocity, as well as the velocity versus the acceleration. Observing Figure A.2, it can be concluded that the modified universal joint exhibits a less smooth behavior when compared with the classical universal joint, which is seen from the fact that the red plot tends to be more scattered than the blue plot. In addition, in the x -direction and z -direction, in general, the results show no substantial differences (see Figure A.2a, Figure A.2b, Figure A.2e and Figure A.2f). However, the most significant differences are observed in the y -direction (see Figure A.2c and Figure A.2d), which agrees with the results previously reported in section 3.5.1 (see Figure 3.25). This phenomenon is associated with the difference on the location of the talocalcaneal joint, which, in turn, is influenced by whether or not the massless link is considered.

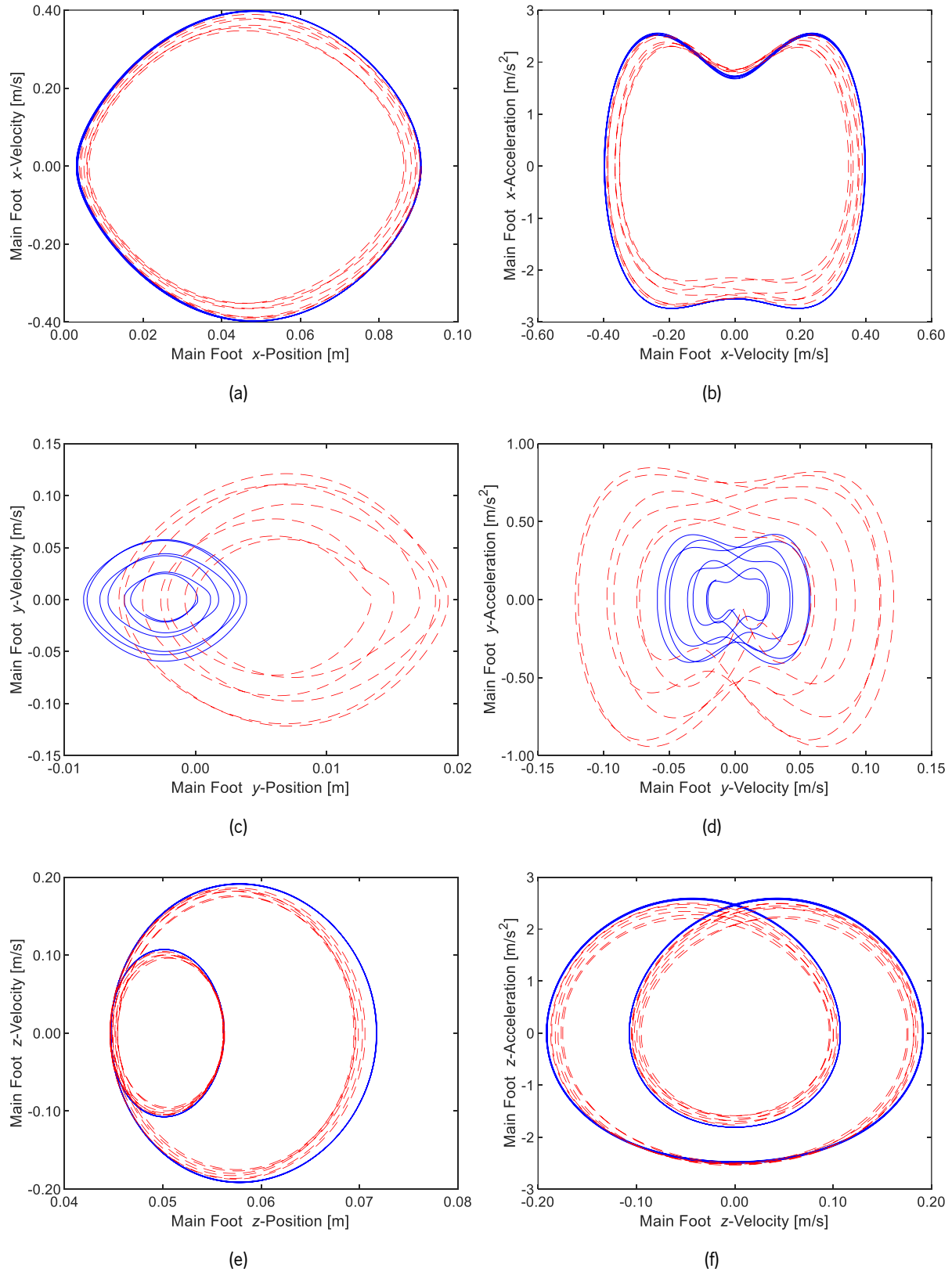


Figure A.2 – Phase portraits of the classical (—) and modified (---) universal joint models: (a) x -position vs. x -velocity, (b) x -velocity vs. x -acceleration, (c) y -position vs. y -velocity, (d) y -velocity vs. y -acceleration, (e) z -position vs. z -velocity and (f) z -velocity vs. z -acceleration.

Appendix B – Time evolution of the joint resistance moments and variation of the mechanical energy of the system

The results presented in this appendix are associated with the analysis carried out in the application example discussed in section 3.5.2. Figure B.1 depicts the evolution of the joint dissipative moment and the evolution of the joint motion-restricting moment for both the talocrural and talocalcaneal joints of the ankle joint complex throughout the simulation time. Since none of the moments are applied to the biomechanical multibody model in both of these joints when the RoM methodology is not considered, this case is not represented in Figure B.1. When the RoM methodology is applied without energy dissipation, only the joint motion-restricting moment is acting on the model. This situation is expected since, with no energy dissipation, the maximum latitude for plantarflexion, inversion and eversion are reached, as discussed in section 3.5.3 (see Figure 3.34 and Figure 3.36). The joint dissipative moment is only applied when energy dissipation is considered in the RoM methodology and its curve and magnitude differ for both joints (see Figure B.1a and Figure B.1b), which is sound because the angular velocity calculated using Eq. (3.131) is different. However, it is important to note that the dissipative moment calculated for the talocrural joint is nearly three times higher than that calculated for the talocalcaneal joint. As observed in Figure B.1b and Figure B.1d, when energy dissipation is considered for the talocalcaneal joint, only the joint dissipative moment is acting on the model, since the maximum latitude for inversion and eversion is not exceeded, as discussed in section 3.5.3 (see Figure 3.34 and Figure 3.36). However, when the RoM is considered with energy dissipation, both moments are acting on the talocrural joint (see Figure B.1a and Figure B.1c). This phenomenon occurs because the maximum latitude for plantarflexion is reached at around 0.43 s of simulation, as observed in Figure 3.36a for $\psi_i=180^\circ$. Since the joint dissipative moment is acting on the model, the relative velocity of the bodies decreases during the simulation. Thus, in the first time the maximum latitude for talocrural plantarflexion is detected, the magnitude of the joint motion-restricting moment is maximum and decreases in subsequent detections, before stabilizing around 0.14 N·m (see Figure B.1c). After stabilization, the model remains in the same configuration for the remainder of the simulation, and, therefore, a constant magnitude of joint motion-restricting moment is applied to prevent the plantarflexion RoM from being exceeded. In general, the application of the joint motion-restricting moment is responsible for the discontinuities observed in the curves of the joint dissipative moment in the plots of Figure B.1a and Figure B.1b. The magnitude of the joint motion-restricting moment is higher than that observed for the joint dissipative moment. However, the former moment is applied in a very short period of time, as opposed to the joint dissipative moment.

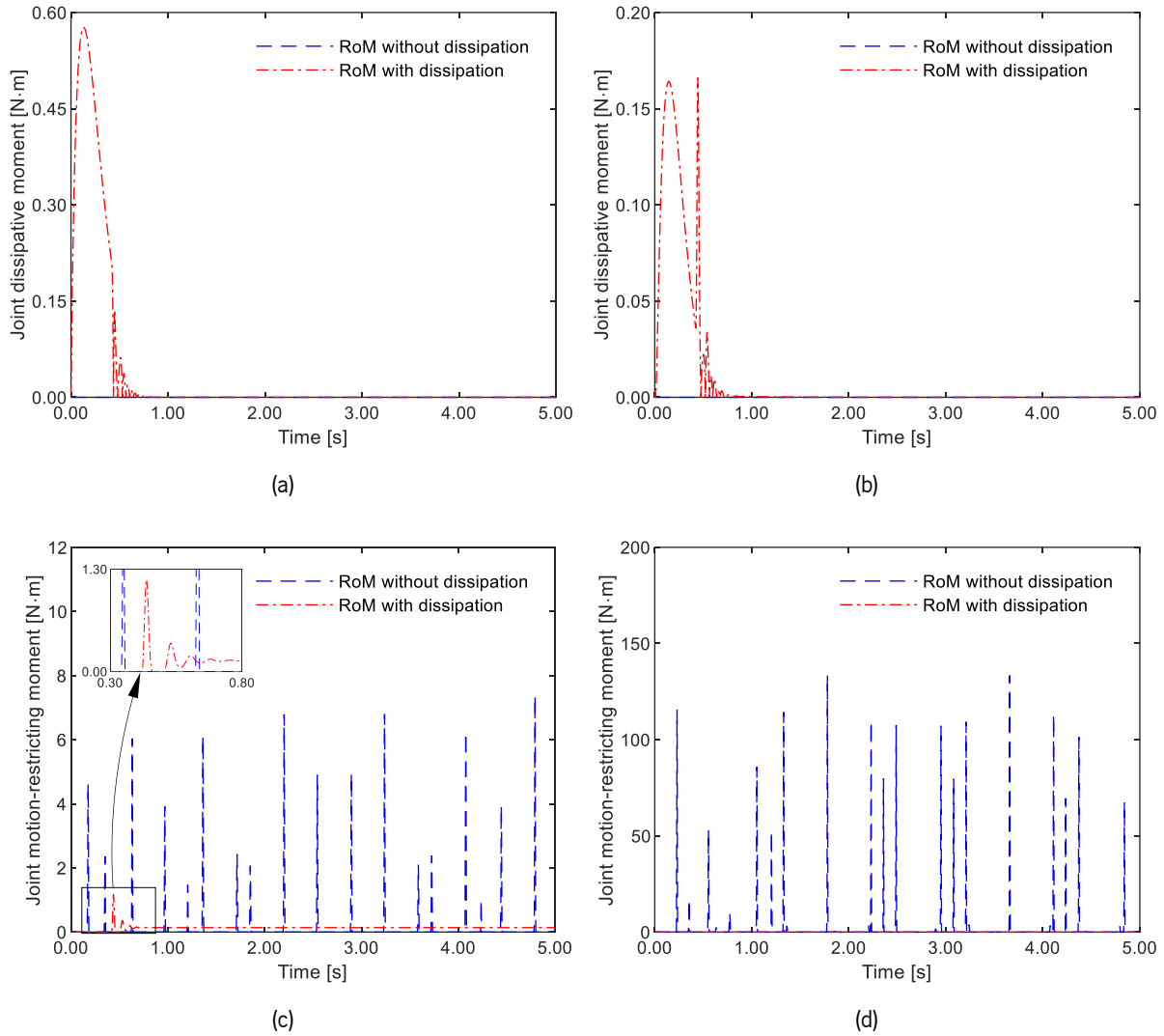


Figure B.1 – Time evolution of the joint dissipative moment for the (a) talocrural and (b) talocalcaneal joints and evolution of the joint motion-restricting moment for the (c) talocrural and (d) talocalcaneal joints throughout the simulation time.

The variation of the mechanical energy of the system is also evaluated, and it is depicted in Figure B.2. If the range of motion methodology is not considered, there is no energy dissipation, and therefore, the system is conservative. If the range of motion methodology is applied without energy dissipation, it can be noted that, whenever the joint motion-restricting moment is applied, which is visible by the peaks present on the plot of the variation of the mechanical energy, the system loses energy. However, the system rapidly recovers since the energy is lost and restored in a short period of time. In this case, the system is conservative. If energy dissipation is considered in the RoM methodology, the system dissipates energy. In addition, the maximum latitude for plantarflexion is reached at around 0.43 seconds. This phenomenon can be observed by the time at which the mechanical energy plateau is reached in the red plot of Figure B.2.

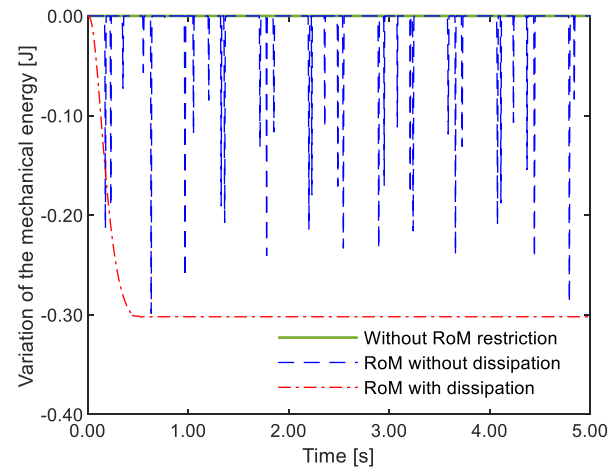


Figure B.2 – Variation of the mechanical energy for the modified universal joint considered to model the ankle joint complex of the human foot.

Appendix C – Validation of the muscle modeling methodology

The analyses conducted in this appendix, which are shown in Figure C.1 and Figure C.2, are associated with the investigation performed in the application example discussed in section 4.5.1.

The observation of the plots (a) and (b) of Figure C.1 and Figure C.2 allow to confirm the conclusions reached in section 4.5.1, regarding the source of the MTU force. Until 1.00 s of simulation, the MTU force observed in Figure 4.20c and Figure 4.20d results exclusively from the action of the contractile element and passive element for the flexor and extensor MTUs, respectively. In turn, from 1.00 s to 2.00 s of simulation the contrary is true. In addition, in Figure C.1c and Figure C.2c, it can be seen that the available contractile element force has a much higher magnitude than the contractile element force that is effectively applied to the double pendulum multibody model for both MTUs (see Figure C.1b and Figure C.2b). This phenomenon occurs because the latter parameter is influenced by the muscle activation, as observed in Eqs. (4.8) and (4.9), which reduce the force the contractile element is capable of exerting. In fact, the available contractile element force is approximately 10 time greater than the force exerted by the contractile element. The observation of plot (e) of Figure C.1 and Figure C.2, allows to infer that the highest magnitude for the force-length relation of the extensor MTU occurs at 0.50 s of simulation, which is in accordance with the time at which it reaches the maximum muscle length (see Figure 4.20e and Figure 4.20f). In turn, the maximum magnitude of the force-length relation for the flexor MTU occurs at 1.50 s of simulation, which also agrees with the results presented in Figure 4.20e and Figure 4.20f.

Regarding the force-velocity relation of the contractile element of Figure C.1f and Figure C.2f, it can be seen that, from 0.00 s to 1.00 s, the magnitude of the flexor/extensor MTU force increases/decreases, until a maximum/minimum value is obtained. At 0.50 s, the magnitude of the force-velocity relation is equal to the maximum isometric force for both MTUs, which is a transition state from concentric to eccentric contraction. At this point, the flexor MTU changes from concentric to eccentric contraction, and the extensor MTU shifts from eccentric to concentric contraction. From 0.00 s to 0.50 s of simulation, the flexor MTU is performing concentric contraction in order to allow flexion of the revolute joint, and the extensor MTU is executing eccentric contraction to control the movement of the bar 2 and prevent excessive acceleration of this body, fulfilling the driving constraint (4.52). From 0.50 s to 1.00 s, the opposite occurs and the extensor MTU performs concentric contraction to allow bar 2 to return to its initial position, and the flexor MTU performs eccentric contraction to decelerate the motion of bar 2. For the remaining simulation time, similar conclusions can be drawn, but with opposite actions. During this period of time, the flexor/extensor MTU performs eccentric/concentric contraction, followed by concentric/eccentric contraction.

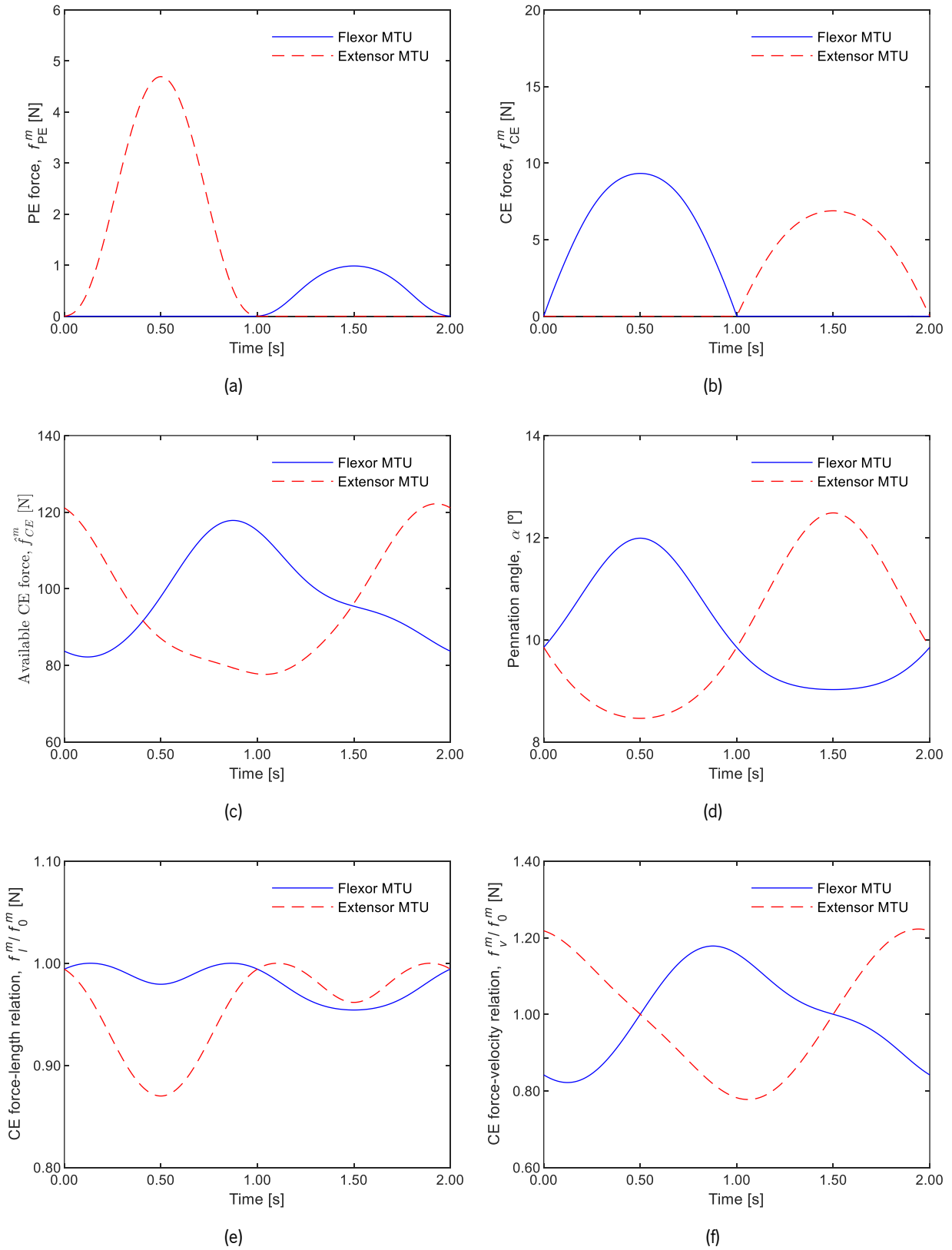


Figure C.1 – Plots for the PE force (a), CE force (b), available CE force (c), pennation angle (d), CE force-length relation (e) and CE force-velocity relation (f) for the model without via-points.

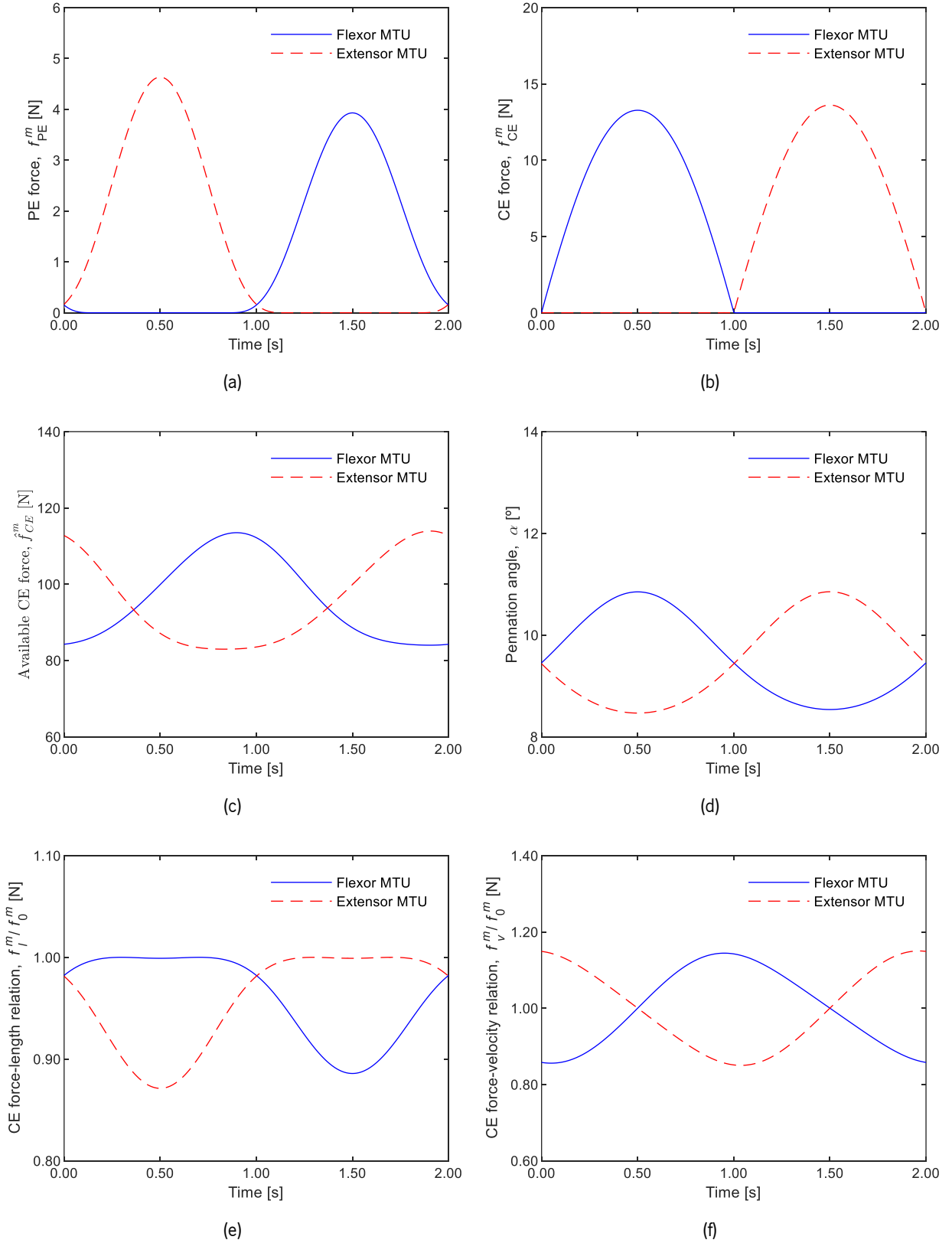


Figure C.2 – Plots for the PE force (a), CE force (b), available CE force (c), pennation angle (d), CE force-length relation (e) and CE force-velocity relation (f) for the model with one via-point.

Figure C.3 depicts the muscle activation patterns obtained using different cost functions for the double pendulum multibody model. It can be concluded that no significant differences are observed in muscle activations the resulting from the use of cost functions (4.44)-(4.46).

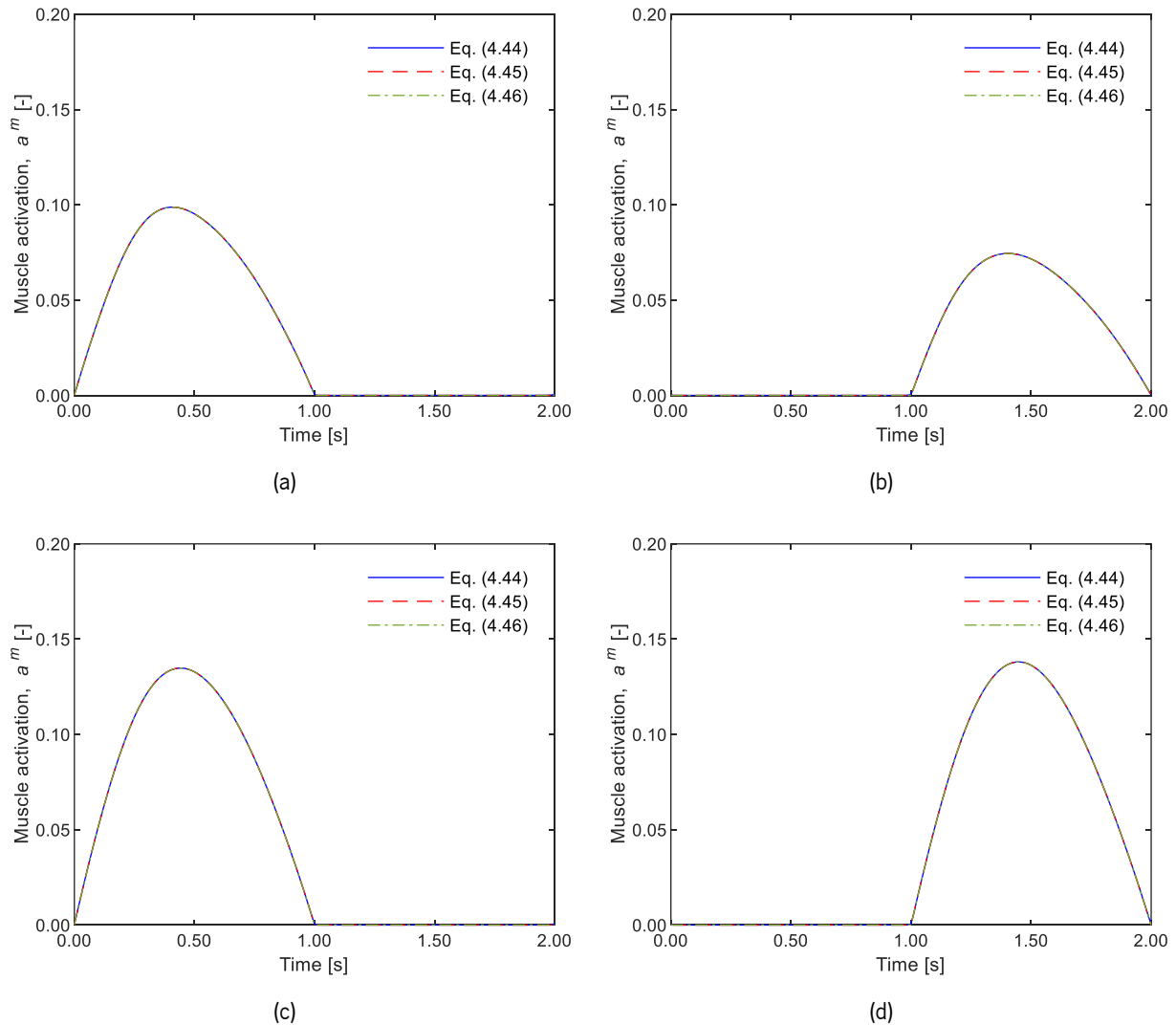


Figure C.3 – Comparison of different cost functions utilized to determine the muscle activations of the flexor (a, c) and extensor (b, d) MTUs in the model without via-points (a, b) and model with one via-point (c, d).

Appendix D – Physiological and geometric parameters of muscles

The physiological and geometric parameters of the muscles considered in this work to control the degrees-of-freedom of the ankle joint complex were taken from the work of Rajagopal et al. (2016). The parameters include the optimal muscle length (l_0^m), tendon length (l^t), maximum isometric muscle force (f_0^m), maximum contractile velocity (v_0^m), muscle pennation angle (α) and the Cartesian coordinates indicating the location of the origin (o), insertion (i) and via-points (v_p). These coordinates are provided with respect to the local reference frames of the bodies of the biomechanical multibody model. However, besides being based on cadaver studies and magnetic resonance imaging muscle volume data (Rajagopal et al., 2016), the parameters reflect the anthropometric characteristics of a 75 kg and 170 cm tall male subject. These dimensions are different from the ones of the subject under analysis in this work (53 kg, 162 cm, female subject), which may significantly affect the prediction of the muscle contributions to a given movement. Hence, in order to improve the similarities of the muscle data with respect to the body of the subject being examined and to avoid inaccurate results, the physiological and geometric parameters of the muscles from Rajagopal et al. (2016) were scaled to the subject. The application of scaling procedures is, up to the present, the most feasible and simple solution of adapting and fitting the physiological and geometric parameters of muscles onto the anatomy of each subject.

In this work, the maximum isometric muscle force and the pennation angle were not scaled and the values of Rajagopal et al. (2016) were utilized. The remaining parameters were scaled by calculating non-dimensional scaling factors. The tendon length was scaled based on the length of the body on which the muscle origin is defined. For instance, the tibialis anterior has origin and two via-points in the leg, and insertion in the main foot. Thus, the scaling factor, κ , for the tendon length is as

$$\kappa_{l^{t,tibant}} = \frac{l_{Rj}^{t,tibant}}{l_{Rj}^{leg}} \quad (D.1)$$

where l_{Rj}^{leg} is the leg length. The subscript “ Rj ” denotes the data taken from Rajagopal et al. (2016).

Concerning the optimal muscle length, if the values provided by Rajagopal et al. (2016) were scaled and considered in the model, $l^m/l_0^m > 1.5$ for all muscles, which significantly compromised the force generating capacity of the contractile element (see Figure 4.10). Hence, the optimal muscle length of each muscle was assumed to be the length calculated using the static trial as the prescribed motion to the biomechanical model. The scaling factor for this parameter was then obtained similarly to Eq. (D.1), that is, the muscle length data from the static trial was scaled by the body length. Also, as stated in section 4.2, $v_0^m = 10l_0^m$, and, therefore, v_0^m is automatically scaled due to the scaling of the l_0^m .

The location of the points utilized to define the muscle was scaled based on the length of the body on which the point is defined. For example, for the tibialis anterior muscle, the following scaling factors were calculated for the origin, first and second via-points, and insertion, respectively

$$\mathbf{K}_{o_{tibant}} = \frac{\mathbf{s}_{leg,Rj}^{o}}{l_{Rj}^{leg}} \quad (D.2)$$

$$\mathbf{K}_{v_1_{tibant}} = \frac{\mathbf{s}_{leg,Rj}^{v_1}}{l_{Rj}^{leg}} \quad (D.3)$$

$$\mathbf{K}_{v_2_{tibant}} = \frac{\mathbf{s}_{leg,Rj}^{v_2}}{l_{Rj}^{leg}} \quad (D.4)$$

$$\mathbf{K}_{i_{tibant}} = \frac{\mathbf{s}_{mainfoot,Rj}^i}{l_{Rj}^{mainfoot}} \quad (D.5)$$

in which the vector $\mathbf{s}_k^P$ represents the coordinates of the point P on the body k local coordinate system.

Table D.1 contains the scaling factors for the physiological and geometric parameters of the muscles considered in this work to control the degrees-of-freedom of the ankle joint complex. It is important to note that for the maximum isometric muscle force and the muscle fiber pennation angle no scaling factors are available because these parameters were not scaled. Hence, the values given in the work of Rajagopal et al. (2016) are presented in Table D.1. The remaining parameters are linearly scaled by the body length, l^b . In addition, Rajagopal et al. (2016) defined both gastrocnemius using the wrap around methodology, which is not considered in the present work. Hence, one via-point, v_1 , was defined for each of those muscles in the location where wrapping occurs using the OpenSim model.

Table D.1 – Scaling factors for the physiological and geometric parameters of muscles

	Name: Soleus								
	Origin: Soleal line of the tibia and posterior surface of proximal fibula								
	Insertion: Converges with both gastrocnemius to form the Achilles tendon, which inserts onto the posterior surface of the calcaneus								
	Action: Plantarflexion								
	f_0^m [N]	α [°]	$\frac{l_0^m}{l^b}$ [-]	$\frac{l^t}{l^b}$ [-]	Points (nr.)	Body (b)	$\frac{\xi}{l^b}$ [-]	$\frac{\eta}{l^b}$ [-]	$\frac{\zeta}{l^b}$ [-]
	6195	21.9	0.1785	0.6917	o (1)	Leg	-0.0200	-0.0250	0.2367
			$(b - leg)$	$(b - leg)$	i (2)	Main Foot	-0.5369	0.0280	0.0056
					i^* (2)	Main Foot	-0.6532	0.0280	0.0056
Note: the symbol “*” indicates the corrected scaling factor for the location of the insertion point									



Name: Gastrocnemius medial head

Origin: Medial femoral condyle

Insertion: The medial and lateral heads of the gastrocnemius combine into a broad aponeurosis which converges with the soleus to form the Achilles tendon

Action: Plantarflexion

f_0^m [N]	α [°]	$\frac{l_0^m}{l^b}$ [-]	$\frac{l^t}{l^b}$ [-]	Points (nr.)	Body (b)	$\frac{\xi}{l^b}$ [-]	$\frac{\eta}{l^b}$ [-]	$\frac{\zeta}{l^b}$ [-]
3116	9.50	0.2763	0.9771	o (1)	Thigh	0.0196	0.0515	-0.5122
		($b - thigh$)	($b - thigh$)	u (2)	Thigh	-0.1447	0.0468	-0.7114
				i (3)	Main Foot	-0.5369	0.0280	0.0056
				i^* (3)	Main Foot	-0.6532	0.0280	0.0056

Note: the symbol “*” indicates the corrected scaling factor for the location of the insertion point



Name: Gastrocnemius lateral head

Origin: Lateral femoral condyle

Insertion: The medial and lateral heads of the gastrocnemius combine into a broad aponeurosis which converges with the soleus to form the Achilles tendon

Action: Plantarflexion

f_0^m [N]	α [°]	$\frac{l_0^m}{l^b}$ [-]	$\frac{l^t}{l^b}$ [-]	Points (nr.)	Body (b)	$\frac{\xi}{l^b}$ [-]	$\frac{\eta}{l^b}$ [-]	$\frac{\zeta}{l^b}$ [-]
1575	12.0	0.2967	0.9216	o (1)	Thigh	-0.0074	-0.0686	-0.5171
		($b - thigh$)	($b - thigh$)	u (2)	Thigh	-0.1303	-0.0765	-0.7239
				i (3)	Main Foot	-0.5369	0.0280	0.0056
				i^* (3)	Main Foot	-0.6532	0.0280	0.0056

Note: the symbol “*” indicates the corrected scaling factor for the location of the insertion point



Name: Tibialis Posterior

Origin: Posterior surface and interosseous membrane of the tibia and fibula

Insertion: Navicular and medial cuneiform

Action: Plantarflexion and inversion

f_0^m [N]	α [°]	$\frac{l_0^m}{l^b}$ [-]	$\frac{l^t}{l^b}$ [-]	Points (nr.)	Body (b)	$\frac{\xi}{l^b}$ [-]	$\frac{\eta}{l^b}$ [-]	$\frac{\zeta}{l^b}$ [-]
1730	13.0	0.1847	0.7017	o (1)	Leg	-0.0100	-0.0250	0.1417
		($b - leg$)	($b - leg$)	u (2)	Leg	-0.0400	0.0450	-0.4456
				u (3)	Main Foot	-0.3244	0.1622	0.0168
				i (4)	Main Foot	-0.1286	0.1566	-0.0783



Name: Tibialis Anterior

Origin: Lateral surface of tibia

Insertion: Medial cuneiform and first metatarsal

Action: Dorsiflexion and inversion

f_0^m [N]	α [°]	$\frac{l_0^m}{l^b}$ [-]	$\frac{l^t}{l^b}$ [-]	Points (nr.)	Body (b)	$\frac{\xi}{l^b}$ [-]	$\frac{\eta}{l^b}$ [-]	$\frac{\zeta}{l^b}$ [-]
1227	11.2	0.2691	0.6010	o (1)	Leg	0.0375	-0.0400	0.1392
		$(b - leg)$	$(b - leg)$	v (2)	Leg	0.0625	-0.0325	-0.0107
				v (3)	Leg	0.0575	0.0325	-0.4481
				i (4)	Main Foot	0.0951	0.1678	-0.0671

Name: Flexor Digitorum Longus

Origin: Medial side of posterior surface of the tibia

Insertion: Plantar surfaces of the 2nd to 5th toes

Action: Plantarflexion and inversion; Flexion of the 2nd to 5th toes



f_0^m [N]	α [°]	$\frac{l_0^m}{l^b}$ [-]	$\frac{l^t}{l^b}$ [-]	Points (nr.)	Body (b)	$\frac{\xi}{l^b}$ [-]	$\frac{\eta}{l^b}$ [-]	$\frac{\zeta}{l^b}$ [-]
423	12.9	0.1975	0.9466	o (1)	Leg	-0.0050	0.0050	0.0092
		$(b - leg)$	$(b - leg)$	v (2)	Leg	-0.0450	0.0300	-0.4431
				v (3)	Main Foot	-0.3132	0.1566	0.0112
				v (4)	Main Foot	-0.1622	0.1454	-0.0671
				v (5)	Main Foot	0.3691	-0.0671	-0.2125
				v (6)	Toes	-0.4014	-0.3564	-0.1535
				v (7)	Toes	-0.0614	-0.4222	-0.1426
				i (8)	Toes	0.1031	-0.4551	-0.1316

Name: Flexor Hallucis Longus

Origin: Posterior surface of the fibula

Insertion: Plantar surface of the phalanx of the great toe

Action: Plantarflexion and inversion; Flexion of the great toe



f_0^m [N]	α [°]	$\frac{l_0^m}{l^b}$ [-]	$\frac{l^t}{l^b}$ [-]	Points (nr.)	Body (b)	$\frac{\xi}{l^b}$ [-]	$\frac{\eta}{l^b}$ [-]	$\frac{\zeta}{l^b}$ [-]
908	14.8	0.2185	0.8856	o (1)	Leg	-0.0775	-0.0500	-0.0732
		$(b - leg)$	$(b - leg)$	v (2)	Leg	-0.0600	0.0200	-0.4506
				v (3)	Main Foot	-0.3523	0.1342	-0.0112
				v (4)	Main Foot	0.0224	0.1454	-0.1286
				v (5)	Main Foot	0.4082	0.1510	-0.1957
				v (6)	Toes	-0.2149	0.0932	-0.1316
				i (7)	Toes	0.2347	0.0055	-0.1755



Name: Extensor Digitorum Longus

Origin: Lateral surface of the tibia and the medial surface of the fibula

Insertion: Distal and middle phalanges of 2nd to 5th toes

Action: Dorsiflexion and eversion; Extension of the 2nd to 5th toes

f_0^m [N]	α [°]	$\frac{l_0^m}{l^b}$ [-]	$\frac{l^t}{l^b}$ [-]	Points (nr.)	Body (<i>b</i>)	$\frac{\xi}{l^b}$ [-]	$\frac{\eta}{l^b}$ [-]	$\frac{\zeta}{l^b}$ [-]
603	12.5	0.2609 (<i>b - leg</i>)	0.9219 (<i>b - leg</i>)	<i>o</i> (1)	Leg	-0.0400	-0.0525	0.1767
				<i>u</i> (2)	Leg	0.0400	-0.0275	-0.4731
				<i>u</i> (3)	Main Foot	-0.0447	-0.0056	0.0336
				<i>u</i> (4)	Main Foot	0.3467	-0.0727	-0.1398
				<i>u</i> (5)	Toes	-0.3794	-0.3564	-0.0110
				<i>i</i> (6)	Toes	0.1031	-0.4661	-0.0658



Name: Extensor Hallucis Longus

Origin: Medial surface of the fibula

Insertion: Base of the distal phalanx of the great toe

Action: Dorsiflexion and inversion; Extension of the great toe

f_0^m [N]	α [°]	$\frac{l_0^m}{l^b}$ [-]	$\frac{l^t}{l^b}$ [-]	Points (nr.)	Body (<i>b</i>)	$\frac{\xi}{l^b}$ [-]	$\frac{\eta}{l^b}$ [-]	$\frac{\zeta}{l^b}$ [-]
286	11.3	0.2937 (<i>b - leg</i>)	0.8167 (<i>b - leg</i>)	<i>o</i> (1)	Leg	-0.0350	-0.0475	0.0792
				<i>u</i> (2)	Leg	0.0175	-0.0400	-0.2607
				<i>u</i> (3)	Leg	0.0500	0.0075	-0.4556
				<i>u</i> (4)	Main Foot	-0.0168	0.1174	0.0503
				<i>u</i> (5)	Main Foot	0.1622	0.1454	0.0056
				<i>u</i> (6)	Main Foot	0.4082	0.1566	-0.0895
				<i>u</i> (7)	Toes	-0.0504	0.0822	-0.0219
				<i>i</i> (8)	Toes	0.2347	0.0164	-0.0329



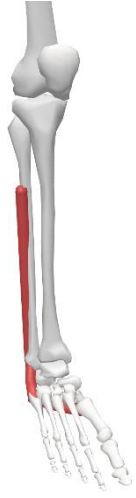
Name: Peroneus Brevis

Origin: Lateral surface of the fibula

Insertion: 5th metatarsal

Action: Plantarflexion and eversion

f_0^m [N]	α [°]	$\frac{l_0^m}{l^b}$ [-]	$\frac{l^t}{l^b}$ [-]	Points (nr.)	Body (<i>b</i>)	$\frac{\xi}{l^b}$ [-]	$\frac{\eta}{l^b}$ [-]	$\frac{\zeta}{l^b}$ [-]
521	11.8	0.2079 (<i>b - leg</i>)	0.3687 (<i>b - leg</i>)	<i>o</i> (1)	Leg	-0.0600	-0.0625	-0.1657
				<i>u</i> (2)	Leg	-0.0850	-0.0625	-0.5056
				<i>u</i> (3)	Leg	-0.0725	-0.0625	-0.5331
				<i>u</i> (4)	Main Foot	-0.2964	-0.1286	-0.0168
				<i>i</i> (5)	Main Foot	-0.1790	-0.1901	-0.0447



Name: Peroneus Longus

Origin: Lateral surface of the fibula

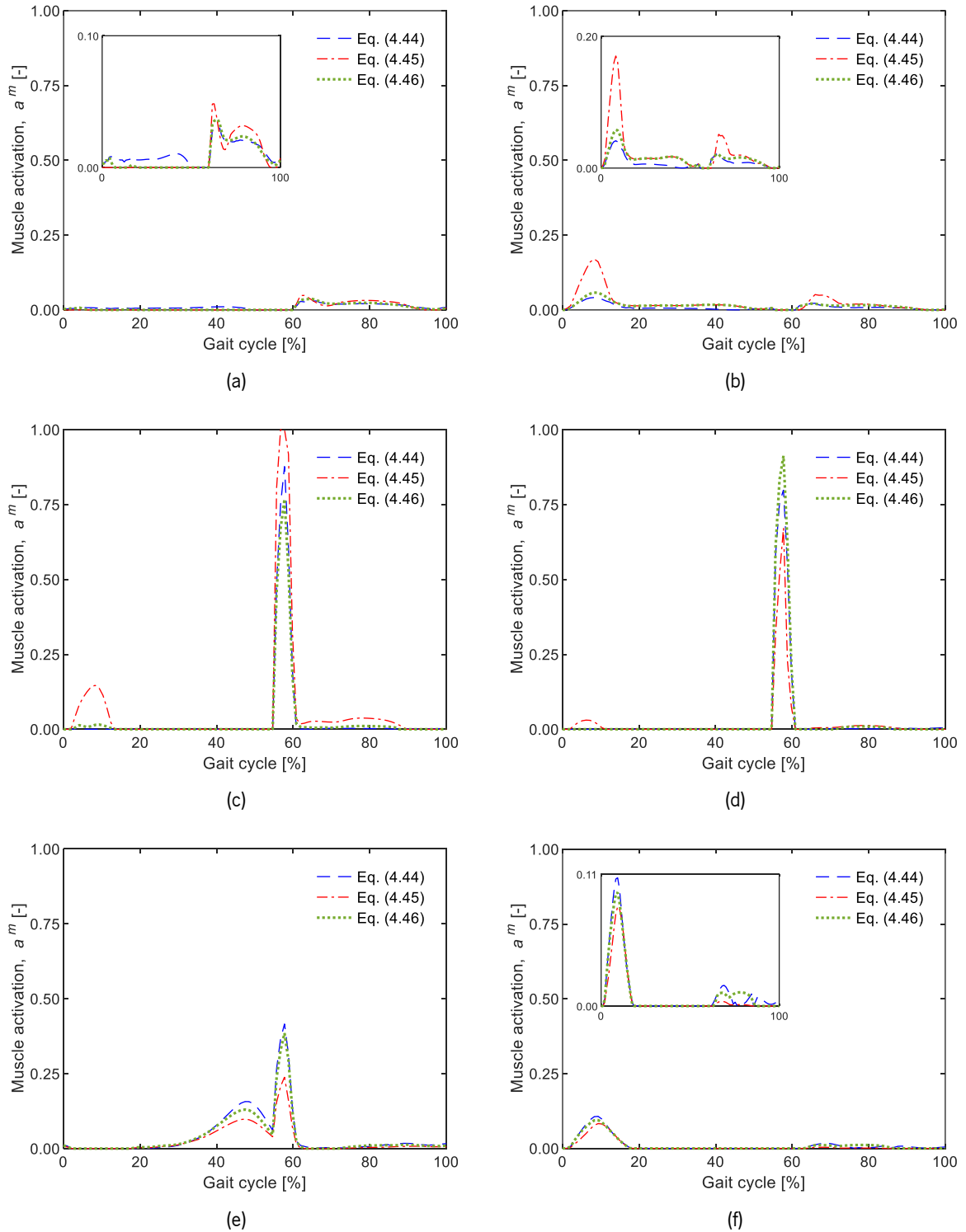
Insertion: Medial cuneiform and base of the 1st metatarsal

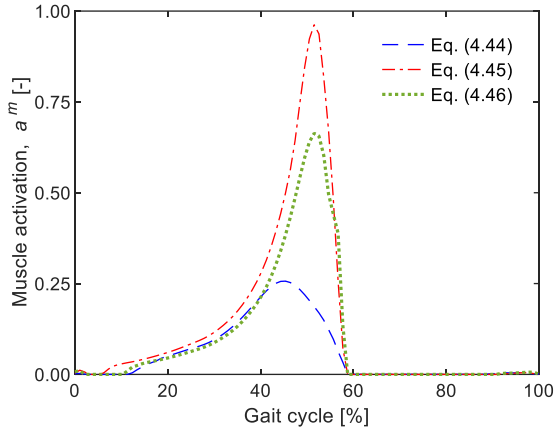
Action: Plantarflexion and eversion

f_0^m [N]	α [°]	$\frac{l_0^m}{l^b}$ [-]	$\frac{l^t}{l^b}$ [-]	Points (nr.)	Body (b)	$\frac{\xi}{l^b}$ [-]	$\frac{\eta}{l^b}$ [-]	$\frac{\zeta}{l^b}$ [-]
1115	14.2	0.2265 ($b - leg$)	0.8303 ($b - leg$)	o (1)	Leg	-0.0500	-0.0700	0.1242
				v_1 (2)	Leg	-0.0800	-0.0600	-0.5081
				v_2 (3)	Leg	-0.0675	-0.0600	-0.5356
				v_3 (4)	Main Foot	-0.3132	-0.1230	-0.0391
				v_4 (5)	Main Foot	-0.1790	-0.1566	-0.1063
				v_5 (6)	Main Foot	-0.0839	-0.0671	-0.1286
				i (7)	Main Foot	0.1118	0.1007	-0.1174

Appendix E – Ankle joint muscle activation patterns, carpet plots, muscle moment arms and muscle moments

The muscle activation patterns of the remaining seven muscles that control the ankle joint complex presented in the application example of section 4.5.2 are illustrated in Figure E.1. The results are related to the model with the adjustment in the insertion of the soleus and gastrocnemius muscles.

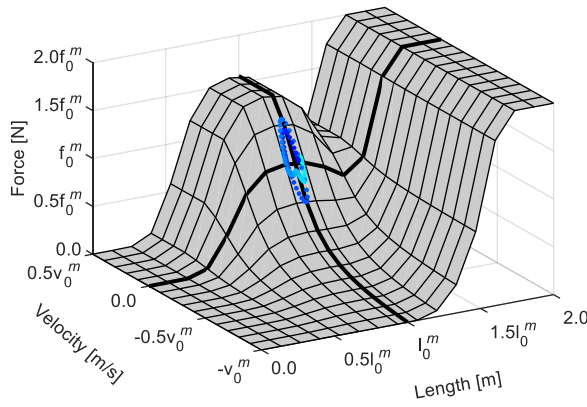




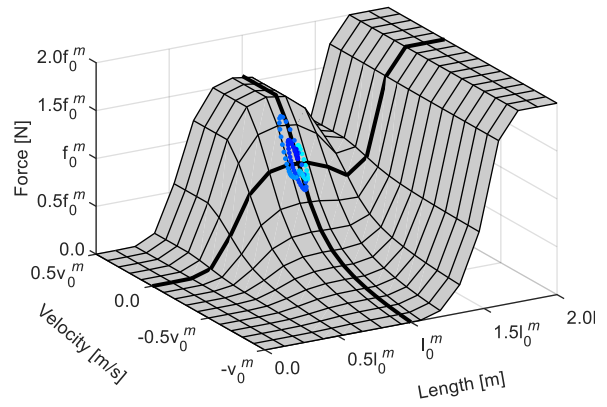
(g)

Figure E.1 – Muscle activations, a^m , for the (a) extensor digitorum longus, (b) extensor hallucis longus, (c) flexor digitorum longus, (d) flexor hallucis longus, (e) peroneus longus, (f) tibialis posterior and (g) medial head of the gastrocnemius muscles. The toe off occurs at 61% of the gait cycle.

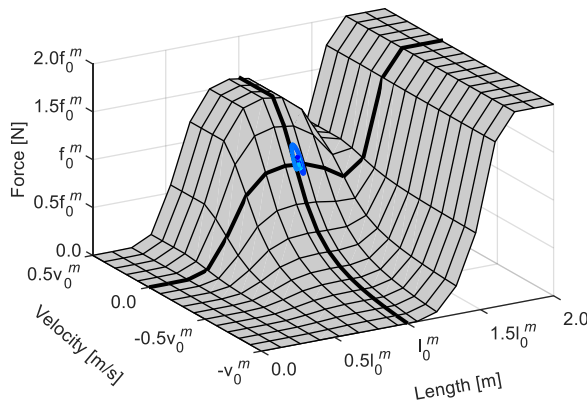
The carpet plots of the remaining seven muscles presented in the application example of section 4.5.2 are illustrated in Figure E.2. The results are obtained using the cost-function represented by Eq. (4.46), since the results for the other two other cost functions, Eqs. (4.44) and (4.45), are identical. The results are related to the model with the adjusted insertion point of the soleus and gastrocnemius muscles



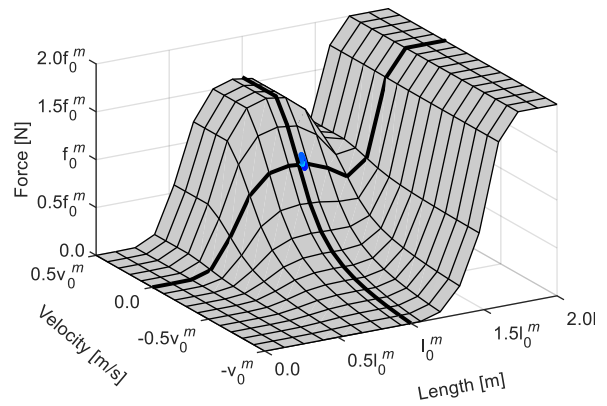
(a)



(b)



(c)



(d)

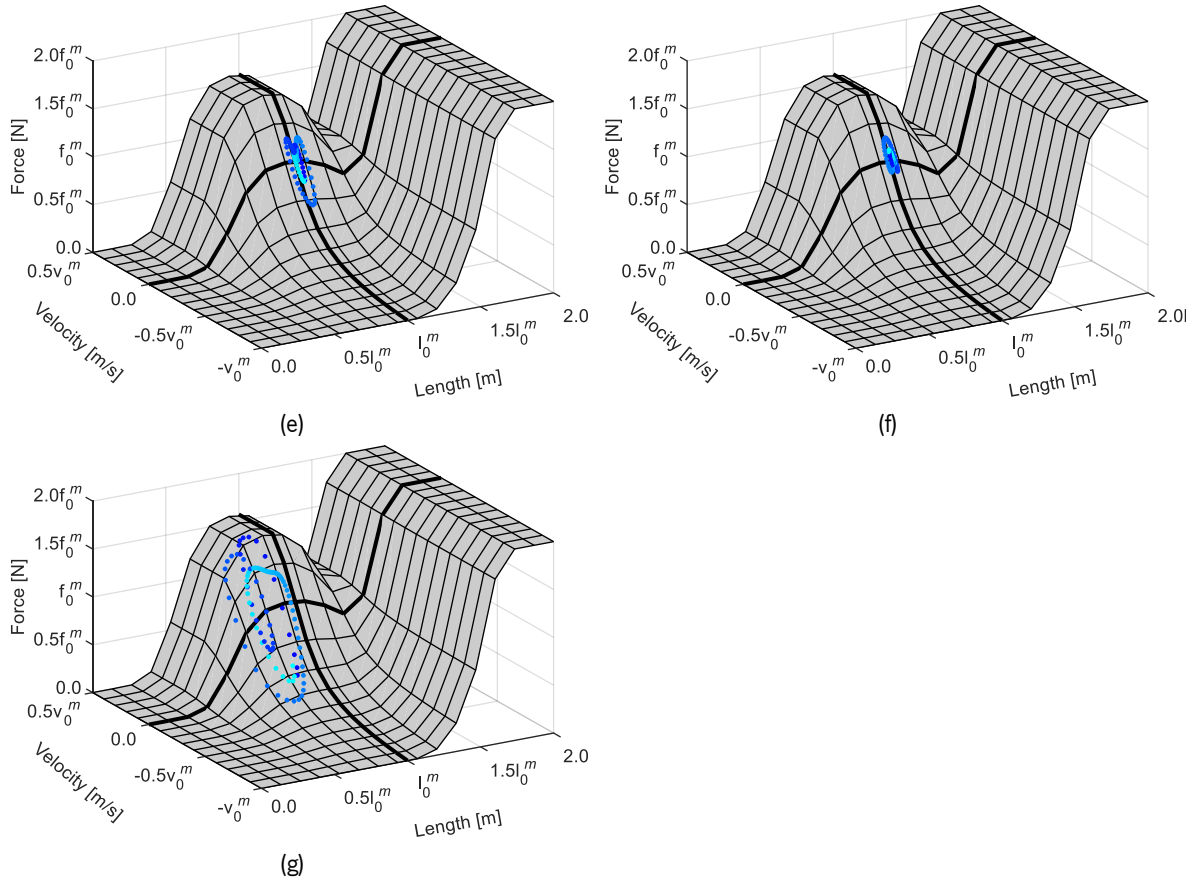


Figure E.2 – Carpet plots for the (a) extensor digitorum longus, (b) extensor hallucis longus, (c) flexor digitorum longus, (d) flexor hallucis longus, (e) peroneus longus, (f) tibialis posterior and (g) medial head of the gastrocnemius muscles.

The moment arms of the muscles utilized in section 4.5.2 were calculated using the following methodology (see Figure E.3). The adopted concept is to find the shortest distance between two vectors, one of them being the vector defining the MTU force and the other being the joint axis vector. First, the vector along the line of action of the MTU force must be calculated using Eq. (4.18) as

$$\mathbf{f}^{mtu} = \mathbf{u}_d f^{mtu} \quad (\text{E.1})$$

A direction unit vector resulting from the cross product of the joint axis vector and the vector calculated in Eq. (E.1) must be determined as

$$\mathbf{n}_i^{mtu} = \frac{\tilde{\mathbf{s}}_i \mathbf{f}^{mtu}}{\|\tilde{\mathbf{s}}_i \mathbf{f}^{mtu}\|} \quad (\text{E.2})$$

where $\mathbf{s}_i$ is the vector defining the axis of joint i . Vector $\mathbf{n}_i^{mtu}$ provides the direction of the moment arm.

Then, the following condition applies

$$\mathbf{d}_i^{mtu} = \mathbf{r}_i^P - \mathbf{r}_{mtu}^Q \quad (\text{E.3})$$

where $\mathbf{r}_i^P$ and $\mathbf{r}_{mtu}^Q$ denote the location of points P and Q on the $\mathbf{s}_i$ joint axis and MTU, respectively. In this work, P was considered to be the point utilized for the definition of the joint and Q was assumed to be either the origin, insertion or via-point of the MTU.

Taking into consideration Eqs. (E.1)-(E.3), then, the moment arm of the MTU can be calculated using the following expression

$$ma^{mtu} = (\mathbf{n}_i^{mtu})^T \mathbf{d}_i^{mtu} \quad (E.4)$$

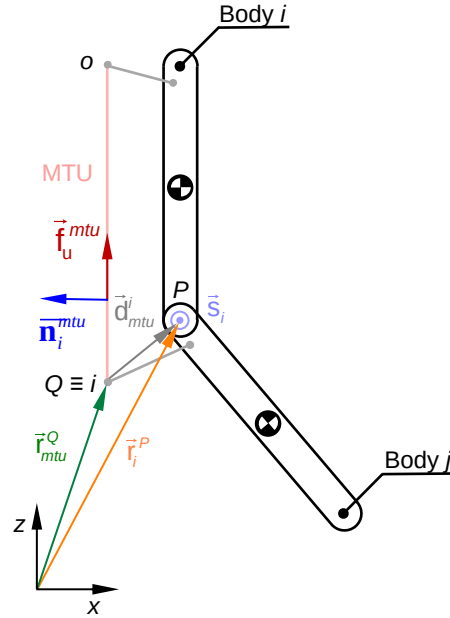


Figure E.3 – Schematic representation of the vectors required for the calculation of the MTU moment arm. The $\mathbf{s}$ joint axis is pointing outwards, thus having the following orientation: [0; -1; 0]. In this example, point Q is the insertion of the MTU.

The moment arms of the muscles utilized in section 4.5.2 are presented in Figure E.4 and Figure E.5. The results are shown for all eleven muscles and for both the plantarflexion/dorsiflexion and inversion/eversion degrees-of-freedom, and, thus, as a function of the talocrural and talocalcaneal joint angles, respectively.

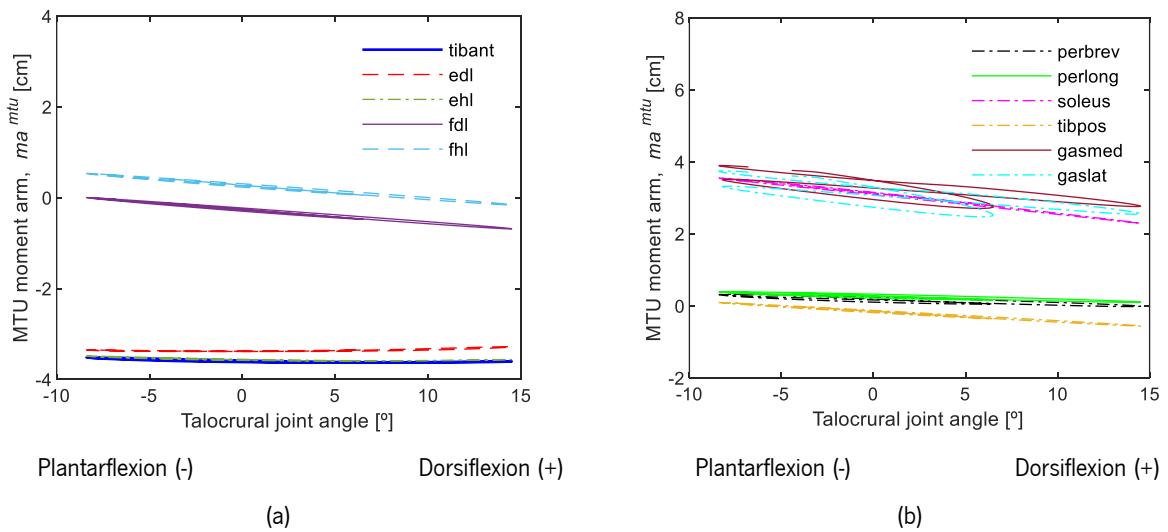


Figure E.4 – Muscle moment arms for the (a) tibialis anterior (tibant), extensor digitorum longus (edl), extensor hallucis longus (ehl), flexor digitorum longus (fdl) and flexor hallucis longus (fhl) muscles, and (b) peroneus brevis (perbrev), peroneus longus (perlong), soleus (soleus), tibialis posterior (tibpos), medial and lateral heads of the gastrocnemius (gasmed, gaslat) muscles. The results are presented as a function of the talocrural joint angle. Positive values for the moment arms indicate plantarflexion.

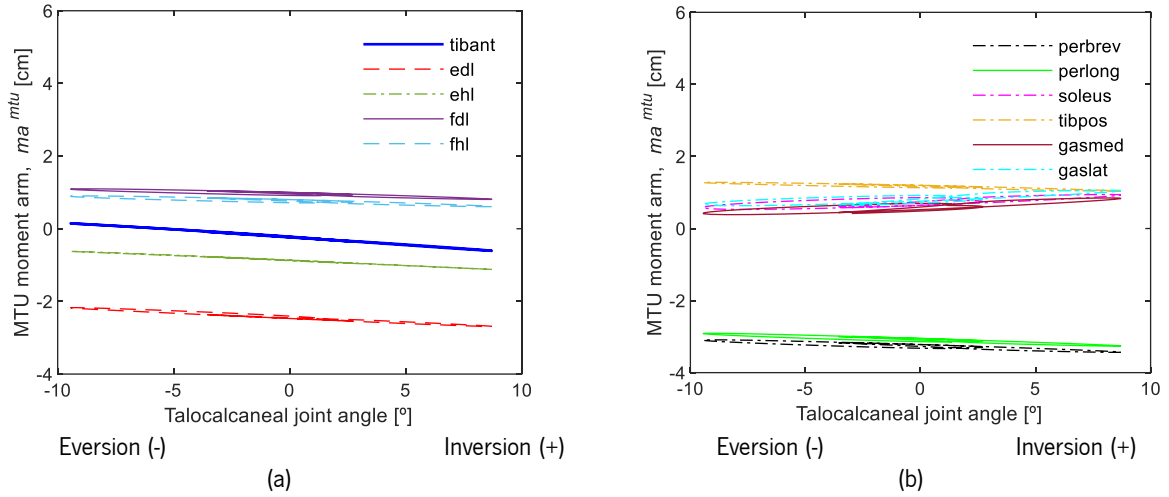
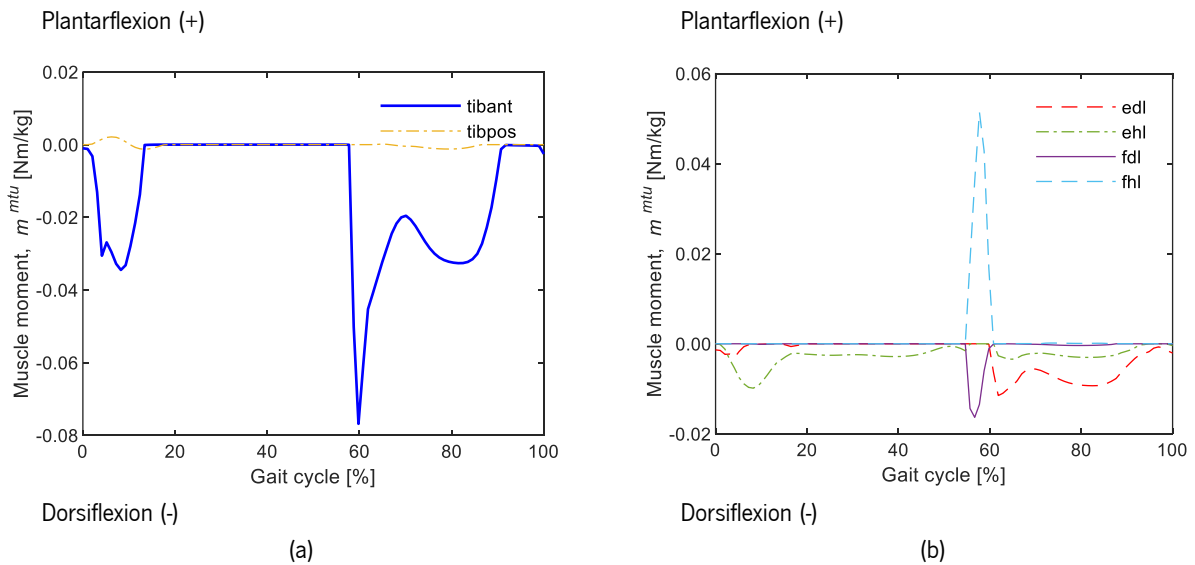


Figure E.5 – Muscle moment arms for the (a) tibialis anterior (tibant), extensor digitorum longus (edl), extensor hallucis longus (ehl), flexor digitorum longus (fdl) and flexor hallucis longus (fhl) muscles, and (b) peroneus brevis (perbrev), peroneus longus (perlong), soleus (soleus), tibialis posterior (tibpos), medial and lateral heads of the gastrocnemius (gasmed, gaslat) muscles. The results are presented as a function of the talocalcaneal joint angle. Positive values for the moment arms indicate inversion.

The MTU moments, m^{mtu} , of the muscles utilized in section 4.5.2 are shown in Figure E.6 and Figure E.7, and are calculated using the MTU force, f^{mtu} , and the moment arm of Eq. (E.4), ma^{mtu} , as

$$m^{mtu} = f^{mtu} ma^{mtu} \quad (E.5)$$

The observation of Figure E.6 and Figure E.7 leads to the conclusion that almost all muscles perform the action specified in Table 4.4 of section 4.5.2. The exception for the talocrural joint is the flexor digitorum longus, which should allow a plantarflexion moment but performs a dorsiflexion moment (see Figure E.6b). In turn, for the talocalcaneal joint, the tibialis anterior (see Figure E.7a) and the extensor hallucis longus (see Figure E.7b) allow an eversion moment, instead of inversion moment. The moments allowed by the muscles around both joints agree the moment arms shown in Figure E.4 and Figure E.5



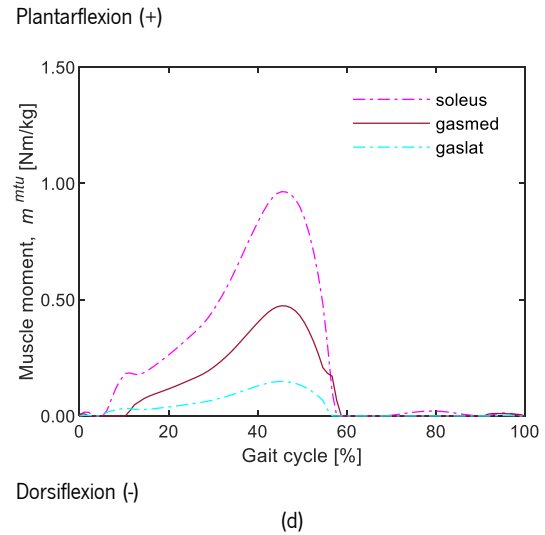
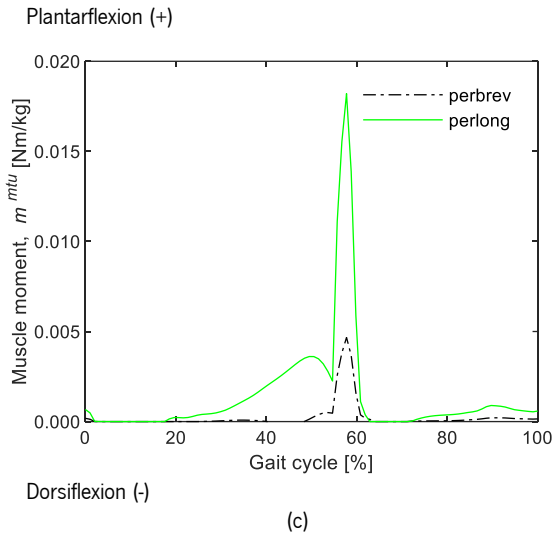


Figure E.6 – Muscle moments around the talocrural joint for the (a) tibialis anterior (tibant) and tibialis posterior (tibpos), (b) extensor digitorum longus (edl), extensor hallucis longus (ehl), flexor digitorum longus (fdl) and flexor hallucis longus (fhl), (c) peroneus brevis (perbrev) and peroneus longus (perlong), and (d) soleus (soleus), and medial and lateral heads of the gastrocnemius (gasmed and gaslat) muscles. The toe off occurs at 61% of the gait cycle.

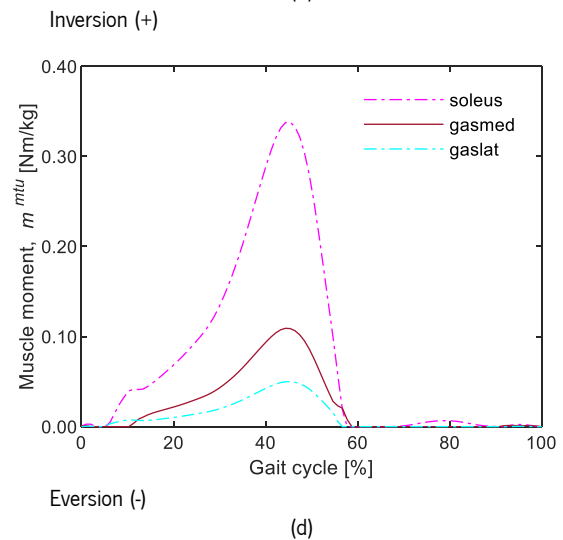
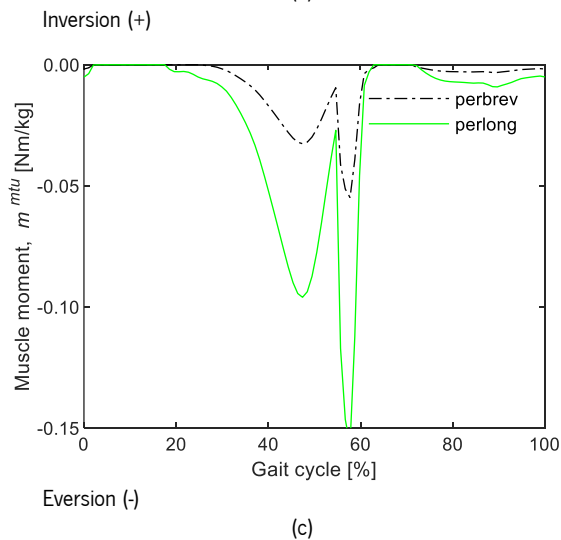
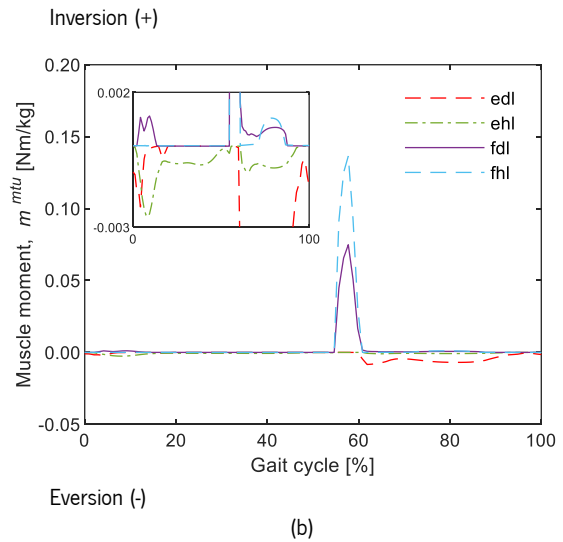
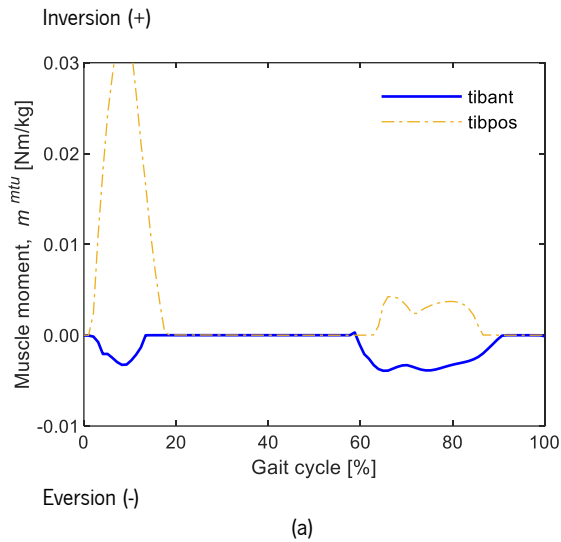


Figure E.7 – Muscle moments around the talocalcaneal joint for the (a) tibialis anterior (tibant) and tibialis posterior (tibpos), (b) extensor digitorum longus (edl), extensor hallucis longus (ehl), flexor digitorum longus (fdl) and flexor hallucis longus (fhl), (c) peroneus brevis (perbrev) and peroneus longus (perlong), and (d) soleus (soleus), and medial and lateral heads of the gastrocnemius (gasmed and gaslat) muscles. The toe off occurs at 61% of the gait cycle.

The talocrural and talocalcaneal joint angles and joint moments throughout the gait cycle are depicted in Figure E.8.

In general, the profile and magnitude of the talocrural joint angle show good agreement with the results reported in the literature (Malaquias et al., 2015; Neumann, 2013; S. Scott & Winter, 1991; Winter, 2009) (see Figure E.8a). It is clear that Figure E.8a presents the two characteristics loading and unloading phases that occur in human gait, which correspond to the two plantarflexion peaks observed at approximately 5% and 65% of the gait cycle, respectively. At the initial support phase (0-5% of gait cycle), the talocrural joint plantarflexes in order to lower the foot towards the ground. When the foot is flat on the ground, the leg starts rotating forward over the foot, provoking dorsiflexion of the talocrural joint (5-50% of gait cycle). Before the toe-off, which occurs at approximately 61% of gait cycle, the talocrural joint plantarflexes, corresponding to the pre-swing phase. During the swing phase of gait, the talocrural joint dorsiflexes in order to prepare the foot for the subsequent gait cycle. The profile and magnitude of the talocrural joint moment is consistent with the literature (Malaquias et al., 2015; Neumann, 2013; S. Scott & Winter, 1991; Winter, 2009) and with the joint angle plot (see Figure E.8c). In the beginning of the gait cycle, a small dorsiflexion moment is generated to control the lowering of the foot to the ground. Then, from 5% to 50% of gait cycle, there is a large plantarflexion moment to control the forward progression of the leg over the foot, which is flat on the ground. Prior to the toe-off, the talocrural joint moment decreases since the corresponding lower limb is unloaded to prepare for the toe-off. During the swing phase of the gait cycle, since no ground reaction forces are acting on the foot, there is a small dorsiflexion moment in order to maintain the talocrural joint dorsiflexed, preventing the toes from touching the ground and ensuring a safe toe clearance.

Throughout the entire duration of the gait cycle, the talocalcaneal joint angle shows similar results to the ones presented in the literature (Maharaj et al., 2017, 2019; S. Scott & Winter, 1991), both in magnitude and profile of the plot (see Figure E.8b). The plot demonstrates that the talocalcaneal joint exhibits inversion at the beginning of the gait cycle, but rapidly transitions to eversion. The joint remains in an everted configuration until approximately 40% of the gait cycle. Prior to the toe off, the joint performs inversion. During the swing phase, both eversion and inversion are allowed. The profile and magnitude of the talocalcaneal joint moment (see Figure E.8d) agree with the literature (Maharaj et al., 2017, 2019; S. Scott & Winter, 1991). In the beginning of the gait cycle, a small eversion moment is generated, followed by a large inversion moment, observed during the majority of the stance phase. These results agree with the joint angle of Figure E.8b. Before the toe-off, the talocalcaneal joint moment gradually decreases, ultimately reaching a value that varies around zero, observed during the swing phase.

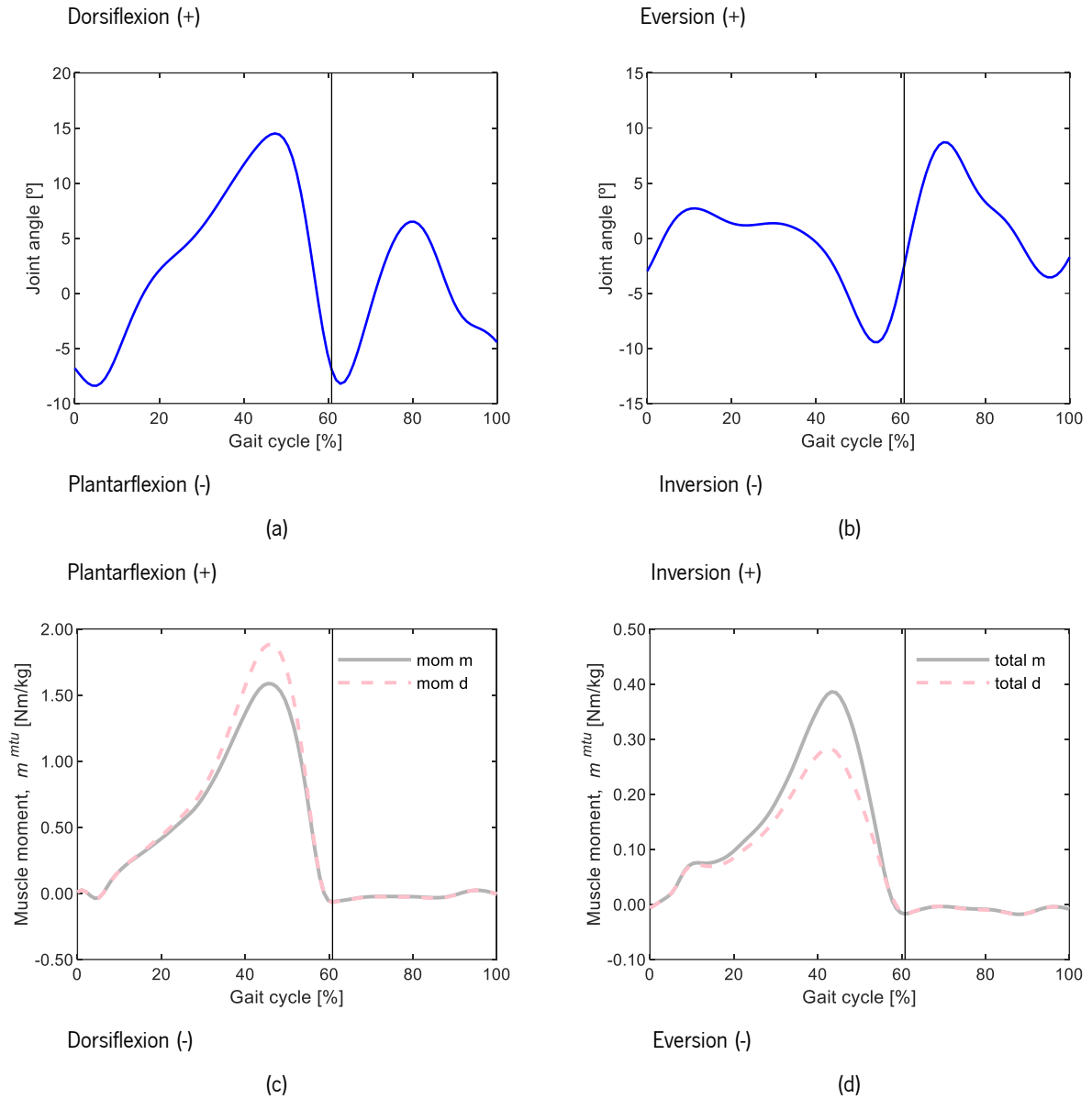


Figure E.8 – Joint angles for the (a) talocrural and (b) talocalcaneal joints, and joint moments for the (c) talocrural and (d) talocalcaneal joints throughout the gait cycle. Joint moment obtained as the sum of the moments of all muscles acting around each joint ($mom\ m$) and joint moment resulting from the joint driver obtained from the same model without muscles ($mom\ d$). The black vertical line indicates the toe off, which occurs at 61% of the gait cycle.

Appendix F – Anthropometric parameters for the biomechanical multibody model

The anthropometric parameters utilized in this work to develop the biomechanical multibody models presented in Chapter 5 include the mass (m_b), length (l_b), moments of inertia (I_b) of each body and the location of the joints with respect to the local coordinate systems of each body, and are based on the data provided by Rajagopal et al. (2016) and Quental (2013). The data given by Quental (2013) is based on the work of Rajagopal et al. (2016), to which some adjustments have been made in order to accommodate the characteristics of the detailed shoulder model, which includes bodies not specified by Rajagopal et al. (2016), namely the clavicle and scapula. The interested reader is referred to the work of Quental (2013) for further details on the performed adjustments. The data from Rajagopal et al. (2016) is utilized for the bodies of the lower limb, which includes the lower trunk, thigh, leg, main foot and toes, while the data from Quental (2013) is considered for the bodies of the upper limb, namely upper trunk, clavicle, scapula, humerus, ulna, radius, and hand. Nevertheless, these data reflect the anthropometric characteristics of a 75 kg and 170 cm tall male subject, which is different from the anthropometry of the subject under analysis in this work (53 kg, 162 cm, female subject). The differences in the anthropometric parameters may significantly affect the performed analyses. Therefore, a scaling procedure is carried out in order to improve the similarities of the data with respect to the body of the subject being examined and to avoid inaccurate results.

In the present work, the considered scaling procedure calculates non-dimensional scaling factors, κ , for each body of the biomechanical model based on the data provided by Rajagopal et al. (2016) and Quental (2013). The mass (m_b) and length (l_b) of each body are scaled using the total mass (m) and height (h) of the subject considering, respectively, the following conditions

$$\kappa_{m_b} = \frac{m_{b,Rj}}{m_{Rj}} \text{ or } \kappa_{m_b} = \frac{m_{b,Q}}{m_Q} \quad (\text{F.1})$$

$$\kappa_{l_b} = \frac{l_{b,Rj}}{h_{Rj}} \text{ or } \kappa_{l_b} = \frac{l_{b,Q}}{h_Q} \quad (\text{F.2})$$

where “ Rj ” and “ Q ” denote the data taken from Rajagopal et al. (2016) and Quental (2013), respectively.

For the main foot and toes, the length scaling factor is calculated using the foot length, l_f , as

$$\kappa_{l_b} = \frac{l_{b,Rj}}{l_{f,Rj}} \quad (\text{F.3})$$

The moments and products of inertia of each body are scaled based on the calculation of the radius of gyration using the following equation (de Leva, 1996)

$$r_b = \frac{1}{\kappa_{l_b} h_{Rj}} \sqrt{\frac{I_{b,Rj}}{m_{Rj} \kappa_{m_b}}} \text{ or } r_b = \frac{1}{\kappa_{l_b} h_Q} \sqrt{\frac{I_{b,Q}}{m_Q \kappa_{m_b}}} \quad (\text{F.4})$$

in which r_b represents the mean relative radius of gyration of body b , κ_{l_b} denotes the scaling factor for the length of body b , h is the total height of the considered subject, I_b is the body b moment or product of inertia, m represents the total mass of the considered subject and κ_{m_b} denotes the scaling factor for the mass of body b .

Table F.1 contains the scaling factors for the anthropometric data utilized on the biomechanical multibody models presented in Chapter 5. All parameters are linearly scaled using Eqs. (F.1)-(F.4).

Table F.1 – Scaling factors for the mass, length and radius of gyration of the biomechanical multibody model

Body	$\frac{l_b}{h}$ [-]	$\frac{l_b}{l_f}$ [-]	$\frac{m_b}{m}$ [-]	Radius of gyration [m]					
				$r_{\xi\xi}$	$r_{\eta\eta}$	$r_{\zeta\zeta}$	$r_{\xi\eta}$	$r_{\xi\zeta}$	$r_{\eta\zeta}$
Lower Trunk ¹	0.0977	-	0.1570	0.5627	0.4223	0.5179	0.0000	0.0000	0.0000
Thigh	0.2400	-	0.1240	0.2940	0.3019	0.1505	0.0000	0.0000	0.0000
Leg	0.2354	-	0.0494	0.2914	0.2934	0.0927	0.0000	0.0000	0.0000
Main Foot	-	0.6623	0.0167	0.1872	0.3203	0.3124	0.0000	0.0000	0.0000
Toes	-	0.3377	0.0029	0.2356	0.7452	0.3332	0.0000	0.0000	0.0000
Upper Trunk ²	0.3984	-	0.3577	0.3462	0.3411	0.2478	0.0000	0.0000	0.0000
Clavicle	0.0791	-	0.0014	0.3105	0.0480	0.3121	0.0000	0.0000	0.0000
Scapula	0.0655	-	0.0105	0.4852	0.4056	0.3248	0.1790	0.0741	0.0589*
Humerus	0.1562	-	0.0271	0.3347	0.3455	0.1511	0.0540*	0.0648	0.0216*
Ulna	0.1431	-	0.0081	0.3033	0.2925	0.1192	0.0217*	0.0325	0.0867
Radius	0.1431	-	0.0081	0.2653	0.2559	0.1042	0.0190*	0.0284	0.0758
Hand	0.0943	-	0.0061	0.3045	0.2795	0.1897	0.0749*	0.1098	0.0998

¹ The “Lower Trunk” body represents the pelvis.

² The “Upper Trunk” body includes the spine, thorax and head.

* The resulting product of inertia is negative.

The locations of the joints of the biomechanical model with respect to the local coordinate system of each body were scaled based on the body length. For instant, the lower trunk is connected to the thigh through the hip joint, and it is also connected to the upper trunk via the back joint. The scaling factors for the location of the hip and back joints on the local reference frame of the lower trunk are as

$$K_{s'} = \frac{S_{lowertrunk}^{hip}}{l_{lowertrunk}} \quad (\text{F.5})$$

$$K_{s'} = \frac{S_{lowertrunk}^{back}}{l_{lowertrunk}} \quad (\text{F.6})$$

Table F.2 provides the scaling factors for the locations of the joints of the biomechanical model with respect to the local coordinate systems of each body.

Table F.2 – Scaling factors for the locations of the joints of the biomechanical model with respect to the local coordinate systems of each body

Joint	Body	Joint location			
		$\frac{\xi}{l^b}$ [-]	$\frac{\eta}{l^b}$ [-] (right side)	$\frac{\eta}{l^b}$ [-] (left side)	$\frac{\zeta}{l^b}$ [-]
Back	Lower Trunk ¹	-0.1807	0.0000	0.0000	0.4908
Hip		0.0869	-0.4653	0.4653	-0.4727
Hip	Thigh	0.0000	0.0000	0.0000	0.4166
Knee		-0.0198	0.0067	-0.0067	-0.5832
Knee	Leg	0.0000	0.0000	0.0000	0.4666
Talocrural		-0.0250	0.0000	0.0000	-0.5331
Talocalcaneal ⁵	Main Foot	-2.1945	0.4423	-0.4423	0.2655
Metatarsophalangeal ⁶		0.5934	-0.0081	0.0081	-0.2410
Metatarsophalangeal ⁷	Toes	-0.1281	-0.0648	0.0648	-0.0222
Glenohumeral	Upper Trunk ²	0.0490	-0.2510	0.2510	0.0760
Sternoclavicular		0.0948	-0.0448	0.0448	0.0767
Back		0.0443	0.0000	0.0000	-0.4725
Sternoclavicular	Clavicle	-0.0082	0.4751	-0.4751	-0.1103
Acromioclavicular		-0.0082	-0.5249	0.5249	-0.1103
Acromioclavicular	Scapula	0.1173	-0.4125	0.4125	0.3144
Scapulothoracic TS ³		0.0399	0.5075	-0.5075	0.1090
Scapulothoracic AI ⁴		0.0075	0.5944	-0.5944	-0.7465
Glenohumeral	Humerus	-0.0171	-0.0260	0.0260	0.4521
Humeroulnar		-0.0171	-0.0260	0.0260	-0.5479
Humeroulnar	Ulna	-0.0097	0.0133	-0.0133	0.3982
Radioulnar		-0.0097	-0.0722	0.0722	0.3982
Radioulnar	Radius	-0.0097	0.0133	-0.0133	0.3983
Radiocarpal		0.0092	0.0898	-0.0898	-0.5986
Radiocarpal	Hand	-0.0409	0.0369	-0.0369	0.4188

¹ The “Lower Trunk” body represents the pelvis.

² The “Upper Trunk” body includes the spine, thorax and head.

³ Scapulothoracic joint on the Trigonum Spinae Scapulae (TS) point.

⁴ Scapulothoracic joint on the Angulus Inferior (AI) point.

⁵ The location of the talocalcaneal joint relative to the main foot local coordinate system is scaled using the talus length.

⁶ The location of the metatarsophalangeal joint relative to the main foot local coordinate system is scaled using the distance from the talocrural joint to the metatarsophalangeal joint.

⁷ The location of the metatarsophalangeal joint relative to the toes local coordinate system is scaled with the total foot length.

The radii, axes and location of the center of the ellipsoid (el) were also scaled based on the length of the upper trunk body, yielding the following scaling factors, respectively

$$\kappa_{el,radii} = [0.0990 \quad 0.1252 \quad 0.2802] \quad (F.7)$$

$$\kappa_{el,axes} = \begin{bmatrix} 0.2181 & 1.4278 & 0.3072 \\ -1.4606 & 0.2112 & 0.0552 \\ 0.0095 & -0.3120 & 1.4433 \end{bmatrix} \quad (F.8)$$

$$\kappa_{el,center,r} = [0.0426 \quad -0.0788 \quad -0.1368] \quad (F.9)$$

$$\kappa_{el,center,l} = [0.0426 \quad 0.0788 \quad -0.1368] \quad (F.10)$$

where the subscripts “ r ” and “ l ” represent the right and left sides, respectively.

Appendix G – Formulation of the ellipsoidal joint

The ellipsoidal joint is specifically formulated for the topology of the upper limb, as described by Quental (2013). The function of this joint is to impose the movement of a point P belonging to a body j to occur over the surface of a body i , which is defined as an ellipsoid. The concept of the ellipsoidal joint is similar to that of the cam-follower joint presented by P. Nikravesh (1988). A schematic representation of a generic ellipsoidal joint is provided in Figure G.1.

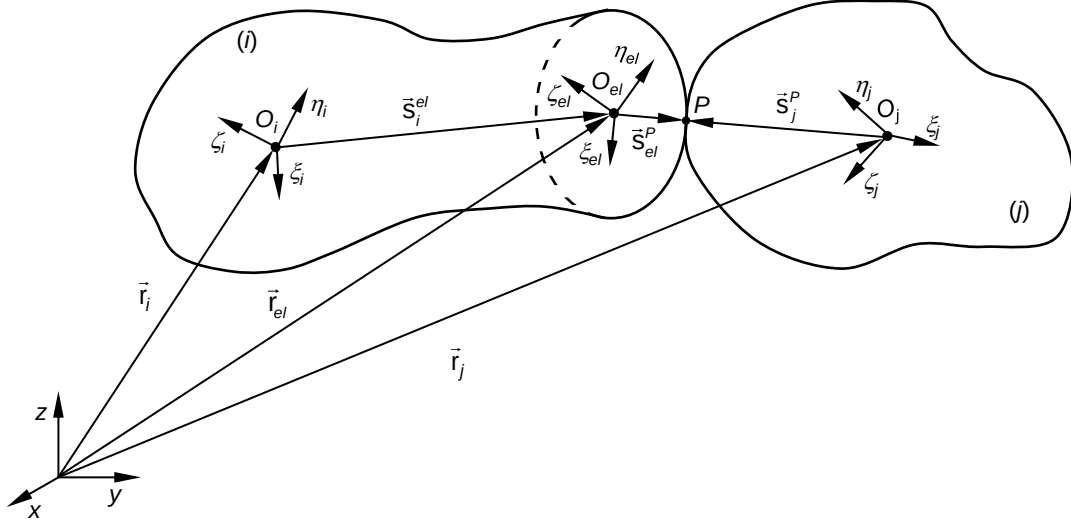


Figure G.1 – Generic configuration of an ellipsoidal joint connecting bodies i and j .

In this work, it is assumed that the body i is the body containing the ellipsoid. Hence, the simplest approach to formulate this joint is to transform the coordinates of a generic point P into the local reference frame of the ellipsoid (el). Observing Figure G.1, the global coordinates of point P can be established as

$$\begin{aligned}
 \mathbf{r}_{el}^P &= \mathbf{r}_j^P \\
 \Leftrightarrow \mathbf{r}_{el} + \mathbf{s}_{el}^P &= \mathbf{r}_j + \mathbf{s}_j^P \\
 \Leftrightarrow \mathbf{s}_{el}^P &= \mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_{el} \\
 \Leftrightarrow \mathbf{s}_{el}^P &= \mathbf{r}_j + \mathbf{s}_j^P - (\mathbf{r}_i + \mathbf{s}_i^{el})
 \end{aligned} \tag{G.1}$$

Applying the condition presented in Eq. (3.21) to Eq. (G.1), then the coordinates of point P expressed in the local reference frame of the ellipsoid are as

$$\begin{aligned}
 \mathbf{s}_{el}^{'P} &= \mathbf{A}_{el}^T (\mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i - \mathbf{s}_i^{el}) \\
 \Leftrightarrow \mathbf{s}_{el}^{'P} &= (\mathbf{A}_i \mathbf{A}_i^{el})^T (\mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i - \mathbf{s}_i^{el}) \\
 \Leftrightarrow \mathbf{s}_{el}^{'P} &= (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i - \mathbf{s}_i^{el}) \\
 \Leftrightarrow \mathbf{s}_{el}^{'P} &= (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i) - (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\mathbf{A}_i \mathbf{s}_i^{el}) \\
 \Leftrightarrow \mathbf{s}_{el}^{'P} &= (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i) - (\mathbf{A}_i^{el})^T \mathbf{s}_i^{el}
 \end{aligned} \tag{G.2}$$

It is important to note that the matrix $\mathbf{A}_i^{el}$ and the vector $\mathbf{s}_i'^{el}$ have constant coordinates in the local reference frame of the ellipsoid.

The ellipsoidal joint allows five relative degrees-of-freedom between the connected bodies and, thus, one kinematic constraint equation must be defined using Eq. (G.2) and the equation of the ellipsoid as (Figure G.1)

$$\Phi^{(el,1)} = \left((\mathbf{s}_{el}'^P)^T \mathbf{R}_{el} \right) \mathbf{s}_{el}'^P - 1 = 0 \quad (G.3)$$

where $\Phi^{(el,1)}$ refers to an ellipsoidal joint constraint with one equation and $\mathbf{R}_{el}$ is a matrix containing the ellipsoid radii, which can be calculated as

$$\mathbf{R}_{el} = \begin{bmatrix} 1/R_{el,\xi}^2 & 0 & 0 \\ 0 & 1/R_{el,\eta}^2 & 0 \\ 0 & 0 & 1/R_{el,\zeta}^2 \end{bmatrix} \quad (G.4)$$

The velocity constraint equation for the ellipsoidal joint is obtained by taking the first time derivative of Eq. (G.3), yielding

$$\dot{\Phi}^{(el,1)} = 2 \left((\mathbf{s}_{el}'^P)^T \mathbf{R}_{el} \right) \dot{\mathbf{s}}_{el}'^P = 0 \quad (G.5)$$

in which the first time derivative of the vector $\mathbf{s}_{el}'^P$ is established as

$$\dot{\mathbf{s}}_{el}'^P = (\mathbf{A}_i^{el})^T \dot{\mathbf{A}}_i^T (\mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i) + (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\dot{\mathbf{r}}_j + \dot{\mathbf{s}}_j^P - \dot{\mathbf{r}}_i) \quad (G.6)$$

Considering the condition expressed in Eq. (3.27), then Eq. (G.6) can be rearranged as

$$\dot{\mathbf{s}}_{el}'^P = (\mathbf{A}_i^{el})^T \dot{\mathbf{A}}_i^T (\mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i) + (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \dot{\mathbf{r}}_i) \quad (G.7)$$

According to P. Nikravesh (1988), the first time derivative of the matrix A is defined as

$$\dot{\mathbf{A}} = \tilde{\boldsymbol{\omega}} \mathbf{A} \quad (G.8)$$

Using Eq. (G.8), then Eq. (G.7) can be reorganized as

$$\begin{aligned} \dot{\mathbf{s}}_{el}'^P &= (\mathbf{A}_i^{el})^T (\tilde{\boldsymbol{\omega}}_i \mathbf{A}_i)^T (\mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i) + (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \dot{\mathbf{r}}_i) \\ \Leftrightarrow \dot{\mathbf{s}}_{el}'^P &= (\mathbf{A}_i^{el})^T \mathbf{A}_i^T \tilde{\boldsymbol{\omega}}_i^T (\mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i) + (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \dot{\mathbf{r}}_i) \end{aligned} \quad (G.9)$$

The transpose of the skew-symmetric matrix of the angular velocity can be expressed as

$$\tilde{\boldsymbol{\omega}}^T = -\tilde{\boldsymbol{\omega}} \quad (G.10)$$

Taking advantage of Eq. (G.10), Eq. (G.9) can be expressed as

$$\begin{aligned} \dot{\mathbf{s}}_{el}'^P &= (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (-\tilde{\boldsymbol{\omega}}_i) (\mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i) + (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \dot{\mathbf{r}}_i) \\ \Leftrightarrow \dot{\mathbf{s}}_{el}'^P &= -(\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\tilde{\boldsymbol{\omega}}_i \mathbf{r}_j + \tilde{\boldsymbol{\omega}}_i \mathbf{s}_j^P - \tilde{\boldsymbol{\omega}}_i \mathbf{r}_i) + (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \dot{\mathbf{r}}_i) \end{aligned} \quad (G.11)$$

Considering Eq. (3.27), then Eq. (G.11) can be rearranged to be expressed in terms of the angular velocity of bodies i and j as

$$\dot{\mathbf{s}}_{el}^{'P} = -(\mathbf{A}_i^{el})^T \mathbf{A}_i^T (-\tilde{\mathbf{r}}_j \boldsymbol{\omega}_i - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_i + \tilde{\mathbf{r}}_i \boldsymbol{\omega}_i) + (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \dot{\mathbf{r}}_i) \quad (\text{G.12})$$

Taking into account the conditions presented in Eqs. (G.5) and (G.12), the contribution of the ellipsoidal joint constraints to the Jacobian matrix can be established as

$$\mathbf{D}^{(el,1)} = 2 \left((\dot{\mathbf{s}}_{el}^{'P})^T \mathbf{R}_{el} \right) \begin{bmatrix} -(\mathbf{A}_i^{el})^T \mathbf{A}_i^T & -(\mathbf{A}_i^{el})^T \mathbf{A}_i^T (-\tilde{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P + \tilde{\mathbf{r}}_i) & (\mathbf{A}_i^{el})^T \mathbf{A}_i^T & -(\mathbf{A}_i^{el})^T \mathbf{A}_i^T \tilde{\mathbf{s}}_j^P \end{bmatrix} \quad (\text{G.13})$$

The formulation of the ellipsoidal joint relies on one kinematic constraint that is not an explicit function of time, and, therefore, vector $\mathbf{v}$ is null.

The time derivative of Eq. (G.5) yields the acceleration constraint equation of the ellipsoidal joint

$$\ddot{\Phi}^{(el,1)} = 2 \left((\dot{\mathbf{s}}_{el}^{'P})^T \mathbf{R}_{el} \right) \dot{\mathbf{s}}_{el}^{'P} + 2 \left((\mathbf{s}_{el}^{'P})^T \mathbf{R}_{el} \right) \ddot{\mathbf{s}}_{el}^{'P} = 0 \quad (\text{G.14})$$

where the second time derivative of the vector $\mathbf{s}_{el}^{'P}$ is expressed as

$$\begin{aligned} \ddot{\mathbf{s}}_{el}^{'P} = & -(\mathbf{A}_i^{el})^T \dot{\mathbf{A}}_i^T (-\tilde{\mathbf{r}}_j \boldsymbol{\omega}_i - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_i + \tilde{\mathbf{r}}_i \boldsymbol{\omega}_i) \\ & -(\mathbf{A}_i^{el})^T \mathbf{A}_i^T (-\tilde{\mathbf{r}}_j \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_j^P + \tilde{\mathbf{r}}_i \dot{\boldsymbol{\omega}}_i - \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{r}}_i) \\ & +(\mathbf{A}_i^{el})^T \dot{\mathbf{A}}_i^T (\dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \dot{\mathbf{r}}_i) + (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\ddot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i) \end{aligned} \quad (\text{G.15})$$

Taking advantage of Eqs. (3.27), (3.31), (G.8) and (G.10) then Eq. (G.15) can be rewritten as

$$\begin{aligned} \ddot{\mathbf{s}}_{el}^{'P} = & (\mathbf{A}_i^{el})^T \mathbf{A}_i^T \tilde{\boldsymbol{\omega}}_i (-\tilde{\mathbf{r}}_j \boldsymbol{\omega}_i - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_i + \tilde{\mathbf{r}}_i \boldsymbol{\omega}_i) \\ & -(\mathbf{A}_i^{el})^T \mathbf{A}_i^T (-\tilde{\mathbf{r}}_j \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \dot{\boldsymbol{\omega}}_i + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_j^P + \tilde{\mathbf{r}}_i \dot{\boldsymbol{\omega}}_i - \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{r}}_i) \\ & -(\mathbf{A}_i^{el})^T \mathbf{A}_i^T \tilde{\boldsymbol{\omega}}_i (\dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \dot{\mathbf{r}}_i) + (\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\ddot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \dot{\boldsymbol{\omega}}_j + \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{s}}_j^P - \ddot{\mathbf{r}}_i) \end{aligned} \quad (\text{G.16})$$

Hence, observing Eqs. (G.14) and (G.16), the contribution of the ellipsoidal joint constraints to the right-hand side vector of the acceleration equations yields

$$\begin{aligned} \gamma^{(el,1)} = & -2 \left((\dot{\mathbf{s}}_{el}^{'P})^T \mathbf{R}_{el} \right) \dot{\mathbf{s}}_{el}^{'P} - 2 \left((\mathbf{s}_{el}^{'P})^T \mathbf{R}_{el} \right) \begin{bmatrix} (\mathbf{A}_i^{el})^T \mathbf{A}_i^T \tilde{\boldsymbol{\omega}}_i (-\tilde{\mathbf{r}}_j \boldsymbol{\omega}_i - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_i + \tilde{\mathbf{r}}_i \boldsymbol{\omega}_i) \\ -(\mathbf{A}_i^{el})^T \mathbf{A}_i^T (\tilde{\boldsymbol{\omega}}_i \dot{\mathbf{r}}_j + \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{s}}_j^P - \tilde{\boldsymbol{\omega}}_i \dot{\mathbf{r}}_i) - (\mathbf{A}_i^{el})^T \mathbf{A}_i^T \tilde{\boldsymbol{\omega}}_i (\dot{\mathbf{r}}_j - \tilde{\mathbf{s}}_j^P \boldsymbol{\omega}_j - \dot{\mathbf{r}}_i) + (\mathbf{A}_i^{el})^T \mathbf{A}_i^T \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{s}}_j^P \end{bmatrix} \end{aligned} \quad (\text{G.17})$$

Taking advantage of Eq. (3.27), then Eq. (G.17) can be rewritten as

$$\begin{aligned} \gamma^{(el,1)} = & -2 \left((\dot{\mathbf{s}}_{el}^{'P})^T \mathbf{R}_{el} \right) \dot{\mathbf{s}}_{el}^{'P} - 2 \left((\mathbf{s}_{el}^{'P})^T \mathbf{R}_{el} \right) \begin{bmatrix} (\mathbf{A}_i^{el})^T \mathbf{A}_i^T \tilde{\boldsymbol{\omega}}_i \tilde{\boldsymbol{\omega}}_i (\mathbf{r}_j + \mathbf{s}_j^P - \mathbf{r}_i) \\ -2(\mathbf{A}_i^{el})^T \mathbf{A}_i^T \tilde{\boldsymbol{\omega}}_i (\dot{\mathbf{r}}_j + \dot{\mathbf{s}}_j^P - \dot{\mathbf{r}}_i) + (\mathbf{A}_i^{el})^T \mathbf{A}_i^T \tilde{\boldsymbol{\omega}}_j \dot{\mathbf{s}}_j^P \end{bmatrix} \end{aligned} \quad (\text{G.18})$$