



Research paper

Kinematic and inverse dynamic analysis using mixed and fully Cartesian coordinates with a generic rigid body

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ABSTRACT

The propagation of errors along a kinematic chain, caused by using drivers computed from noisy data, can affect the accuracy of the kinematic and dynamic outcomes. Minimizing the effect of such errors is crucial, particularly when traditional smoothing techniques prove to be ineffective.

This work expands the multibody formulation with Fully Cartesian Coordinates and a Generic Rigid Body (FCC-GRB) to the inverse dynamic analysis of spatial mechanical systems using mixed coordinates (MC). This method considers the incorporation of angular variables, enabling the determination of the kinematic consistent positions that best fit the reference data, while simultaneously computing the joint angular drivers. The accuracy and computational performance of the formulation are evaluated using both numerical- and optimization-based methods in the study of two mechanisms guided with perturbed data.

The results show that implementing an MC methodology with FCC-GRB can be easily performed without compromising the theoretical foundations of the classical formulation. This approach efficiently computes both the positions and drivers of the model simultaneously, avoiding the propagation of errors along the kinematic chain. Numerical methods based on the Newton-Raphson algorithm generated positions closely matching the reference data, while optimization-based methods ensured a stricter fulfillment of the topological constraints.

1. Introduction

The inverse dynamic analysis of multibody mechanical systems typically requires prior computation of kinematic positions from noisy or missing experimental data [1,2]. A classic example is the biomechanical analysis of human motion. Typically, when acquiring experimental data, a set of reflective markers is placed on the subject's skin at specific locations, often corresponding to bony eminences [3–5]. Due to the relative motion of soft tissues, such as the skin, muscles, tendons, and ligaments, in relation to the bones, a phenomenon usually referred to as soft tissue artifact (STA), the acquired data is prone to experimental errors. These can affect the quality of the measured outcomes, making it challenging to use the data at a clinical level [6–10]. This artifact is particularly difficult to remove from experimental data without relying on specialized real-time medical imaging techniques (e.g., [11–13]), as it often has the same frequency as the movement itself and is task-dependent. For instance, its magnitude, frequency, and timing may vary

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Nomenclature Head

Abbreviations

3D	Three-Dimensional
AR	Angular Relation
CNO	Constrained Nonlinear Optimization
CoM	Center of Mass
DoF	Degree of Freedom
ED	Euclidean Distance
EoM	Equations of Motion
FCC-GRB	Fully Cartesian Coordinates with Generic Rigid Body
KA	Kinematic Analysis
LS	Least Squares
MCR	Mixed Coordinates Relation
MO	Multi-Objective
NRM	Newton-Raphson Method
STA	Soft Tissue Artifact
TC	Tracking Constraint
TOC	Tracking Orientation Constraint
WLS	Weighted Least Squares

Symbol (Latin)

$\mathbf{0}_3, \mathbf{I}_3$	Null and identity matrices
$\mathbf{C}_i^P$	Constant transformation matrix of a generic point P with respect to body i
$\mathbf{C}_i^s$	Constant transformation matrix of a generic vector $\mathbf{s}$ with respect to body i
$\mathcal{C}^{s_1, s_2}$	Constant transformation matrix that relates the generic vectors $\mathbf{s}_1$ and $\mathbf{s}_2$
$F, \mathbf{F}$	Objective function of the optimization problem
$\mathbf{F}_q$	Jacobian matrix of the objective function $\mathbf{F}$
$\mathbf{F}^*$	Optimization goals of the multi-objective goal attainment problem
$\mathbf{g}$	Generalized forces of the system
$\mathbf{g}^\Phi$	Generalized internal forces
$\mathbf{M}$	Mass matrix of the system
nb, nc, nd, n_{TC}	Number of bodies, kinematic constraints, generalized angular variables and tracking constraints of the system
P	Generic point P
P^*	Reference point P^*
O_i	Origin of the local reference frame of body i
$\mathbf{q}, \dot{\mathbf{q}}, \ddot{\mathbf{q}}$	Generalized positions, velocities and accelerations of the system
$\mathbf{q}_{3v_i}, \dot{\mathbf{q}}_{3v_i}, \ddot{\mathbf{q}}_{3v_i}$	Position, velocity and acceleration of the fully-defined equivalent vector of the reduced rigid body i
$\mathbf{q}_{lb}, \mathbf{q}_{ub}$	Lower and upper bounds of the generalized coordinates for the optimization
$\mathbf{q}_n$	Solution a of the NRM for iteration n
$\mathbf{r}_P, \dot{\mathbf{r}}_P, \ddot{\mathbf{r}}_P$	Position, velocity and acceleration vectors of the generic point P in the global reference frame
$\mathbf{r}_{P^*}, \dot{\mathbf{r}}_{P^*}, \ddot{\mathbf{r}}_{P^*}$	Position, velocity and acceleration vectors of a reference point P^* in the global reference frame
$\mathbf{s}, \dot{\mathbf{s}}, \ddot{\mathbf{s}}$	Position, velocity and acceleration vectors of a generic unit vector $\mathbf{s}$
$\mathbf{s}^*, \dot{\mathbf{s}}^*, \ddot{\mathbf{s}}^*$	Position, velocity and acceleration vectors of a reference unit vector $\mathbf{s}^*$
$\mathbf{S}$	Constant transformation matrix that converts the reduced rigid body i in its fully-defined equivalent form
t	Time
$\mathbf{u}_i, \dot{\mathbf{u}}_i, \ddot{\mathbf{u}}_i, \mathbf{v}_i, \dot{\mathbf{v}}_i, \ddot{\mathbf{v}}_i, \mathbf{w}_i, \dot{\mathbf{w}}_i, \ddot{\mathbf{w}}_i$	Position, velocity and acceleration of the generic rigid body vectors $\mathbf{u}, \mathbf{v}$ and $\mathbf{w}$ of body i in the global reference frame
$\bar{\mathbf{V}}_i, \mathbf{V}_i, \dot{\mathbf{V}}_i$	Transformation matrices that convert the reduced rigid body i into its fully-defined equivalent form
w_n	Weight coefficient of the n -th tracking constraint
$\mathbf{w}_{MO}$	Weight coefficients vector for the MO optimization
$\mathbf{W}$	NRM-WLS and optimization weight matrix

Symbol (Greek)

γ	Right-hand-side vector of the acceleration equations of the system
γ^k	Right-hand-side vector of the acceleration equations for the kinematic constraint of type k
Y	Slack variable of the multi-objective goal attainment problem
ε	Newton-Raphson iteration tolerance
$\boldsymbol{\theta}$	Vector of the generalized angular variables
θ_k	k -th angular generalized coordinate of the model

θ_k^*	Reference angle for the k -th angular generalized coordinate of the model
$\theta_{s_1 s_2}$	Angle between two generic unit vectors s_1 and s_2
$\theta_{s_1 s_2}^*, \dot{\theta}_{s_1 s_2}^*, \ddot{\theta}_{s_1 s_2}^*$	Angular position, velocity and acceleration of a reference angle θ^* between two generic unit vectors s_1 and s_2
λ	Lagrange multipliers of the system
λ^k	Lagrange multipliers for the kinematic constraint of type k
ν	Right-hand-side vector of the velocity equations of the system
ν^k	Right-hand-side vector of the velocity equations for the kinematic constraint of type k
τ_k^{int}	Internal joint moment of force associated to joint k
$\Phi, \dot{\Phi}, \ddot{\Phi}$	Vector of the kinematic constraints and respective first derivative and second derivative with respect to time
Φ_q	Jacobian matrix of the system
Φ^k	Kinematic constraint equation of type k
Φ_q^k	Contributions to the Jacobian matrix from the kinematic constraint of type k

depending on the movement being analyzed, the individual's anthropometric characteristics, the body segment and anatomical joint involved, and the muscle activation pattern. As a result, automatic detection becomes difficult, and standard filtering techniques are often ineffective for its attenuation [6,14].

Obtaining high-quality kinematic and kinetic inputs is crucial, as they have a significant influence on the quality of the dynamic outcomes [15]. A common procedure for ensuring the quality of kinematic inputs involves computing the kinematic consistent positions for a given model. Essentially, this procedure determines the positions, velocities, and accelerations of the system that comply with a set of topological constraints, which define mathematically the model, and driving constraints that guide its movement [1].

Methodologies based on multibody system formulations present themselves as an efficient and accurate approach to performing the kinematic and dynamic analysis of complex mechanical models [16]. Two classical approaches are commonly employed to compute the kinematic consistent positions [17]. The first addresses the problem through a forward kinematics approach. The joint angular drivers, which usually describe the angular degrees-of-freedom (DoFs) of the model, are computed from the experimental data in a pre-analysis phase. These drivers are then applied to the model during the kinematic analysis (KA) to determine the position and orientation of all the segments [1,17]. The second method utilizes reference points and vectors to determine the kinematic consistent positions that minimize the differences from these references, following an inverse kinematics approach [17,18]. In order to address the inaccuracies in the experimental data, such as STA, several methods have been proposed. Some of them use specific algorithms designed to mitigate these effects (e.g., [19–21]), while others rely on numerical or optimization methods together with multibody-based models (e.g., [7,9,10,22,23]). The choice of the most appropriate method depends on the desired level of accuracy, movement in analysis, or computational performance requirements.

Several multibody formulations are available in the literature, presenting different advantages and target applications [17,24–31]. Recently, based on the work of Gameiro et al. [32], Roupá et al. [28] and Gonçalves et al. [29] presented the theoretical basis of the Fully Cartesian Coordinates with a Generic Rigid Body (FCC-GRB) formulation for the planar and spatial analysis of multibody systems. Due to the type of coordinates used to describe the system and the kinematic structure adopted to model the segments, this formulation preserves some of the main characteristics reported for the most common global formulations, namely the natural coordinates [17,27,33] and Cartesian coordinates [24–26].

Similarly to the natural coordinates formulation, in the FCC-GRB formulation, the multibody system is described using only rectangular coordinates of points and unit vectors, implying that no angular-related variables are required to describe the orientation of the bodies. Furthermore, the kinematics of any point or vector belonging to the model can be expressed as a linear transformation of a set of constant transformation matrices (matrices C and V) and the generalized coordinates of the system. These features imply that the constraint equations for the most common kinematic constraints present, at the most, a quadratic dependency on the generalized coordinates of the system, and, consequently, the respective contributions to the Jacobian matrix and right-hand side vectors of velocity and acceleration are quadratic, linear, constant, or null [28,29].

Conversely to the natural coordinates formulation, in which the definition of the bodies depends on the topology of the system, the rigid bodies are defined with a predetermined kinematic structure composed of one reference point and two or three unit vectors. Moreover, if the reference point is located at the center of mass (CoM) of the body, the rigid body mass matrices become diagonal with their entries equal to the inertial properties of the segments being modeled [28,29]. The use of a generic rigid body approximates the proposed formulation to the Cartesian coordinates approach. Hence, some of the advantages often associated with this formulation, namely the easier systematization of the modeling procedure, and the straightforwardness and high physical meaning of the mass matrices, also apply to the FCC-GRB formulation, simplifying its computational implementation [28,29].

Some authors explored a hybrid multibody formulation based on natural coordinates, which also uses angular variables [34,35]. This approach, originally proposed by Jalón and Bayo [17], considers that the set of generalized coordinates includes not only the coordinates that define the model topology but also the angular drivers that guide the system, allowing for the simultaneous determination of the consistent positions and orientations of the model and their respective angular DoFs. Due to the hybrid nature of the coordinates that compose the system, this formulation is commonly referred to as mixed coordinates (MC) [17,34,35].

The modeling approach with MC is particularly useful when performing the kinematic analysis of systems that require the prior calculation of input drivers from experimental data, which may be subject to measurement errors. By minimizing the distance between the experimental data and the corresponding elements of the mechanical model (e.g., points, vectors, orientations), this methodology

enables to find the kinematic consistent positions that best fit the input data over time. Furthermore, as the entire position is minimized at the same time, small errors due to data inconsistency are not propagated along the kinematic chain, as in the case of the kinematic analysis with drivers. These advantages are particularly suitable for the biomechanics field, where experimental data is often contaminated with STA, which can result in marker displacements of a few centimeters from their original position [8,9,36]. The use of an MC approach allows for attenuation of the effect of these artifacts, while simultaneously computing the joint angular drivers directly from the experimental markers. In addition, this step eliminates the need for pre-processing procedures that involve the calculation of the three-dimensional (3D) angles from experimental data, which is often a complex issue, especially for users with less expertise in the topic.

Thus, the present work examines the use of an MC approach in tandem with an FCC-GRB formulation to perform the kinematic and inverse dynamic analysis of spatial multibody systems. Three different approaches to solving the kinematic equations are considered, namely the Newton-Raphson iterative method (NRM) together with a weighted least squares (WLS) minimization, a constrained nonlinear optimization (CNO) and a multi-objective (MO) goal attainment optimization, to evaluate their influence on the accuracy of the reconstruction of the kinematic consistent positions from the experimental data, the violation of the kinematic constraints and computational time. With the purpose of assessing its applicability, the FCC-GRB formulation with an MC approach is applied in the analysis of two mechanisms, considering, as inputs, data with and without perturbations.

According to Roupa et al. [28] and Gonçalves et al. [29], one of the major advantages of modeling multibody systems with an FCC-GRB formulation is its ease of implementation and modeling of complex mechanical systems. This fact implies that, in addition to the classical applications usually attributed to the global multibody formulations, the FCC-GRB formulation is suitable for advanced education purposes. As the incorporation of the angular variables does not significantly change the modeling procedure, the straightforwardness reported to the planar and spatial formulation is still applicable in the mixed coordinates variation. Consequently, the steps required to incorporate angular coordinates into the formulation are presented in detail, so that, together with the planar and spatial FCC-GRB studies [28,29], this work can serve as an educational tool for supporting the teaching of multibody-related topics.

2. Formulation

2.1. Fundamental aspects of the FCC-GRB formulation

In the FCC-GRB formulation, multibody systems are modeled using a set of rigid bodies defined with a pre-determined kinematic structure. This approach follows the methodology used in the Cartesian coordinates formulation, presenting advantages in the systematization of the modeling procedure and definition of the system mass matrices. However, contrary to Cartesian coordinates formulation case, which uses angular-related coordinates, the mathematical structure adopted for defining each body uses only rectangular coordinates of points and vectors. Specifically, the structure adopted for the rigid body considers the use of one vector that defines the reference point ($\mathbf{r}_{O_i}$), usually located at its center of mass, and three non-coplanar unit vectors ($\mathbf{u}_i, \mathbf{v}_i, \mathbf{w}_i$), as schematically represented in Fig. 1a. Therefore, the vector of the generalized coordinates for the generic rigid body i ($\mathbf{q}_i$) is defined as [29]

$$\mathbf{q}_i = \{ \mathbf{r}_{O_i}^T \quad \mathbf{u}_i^T \quad \mathbf{v}_i^T \quad \mathbf{w}_i^T \}^T \quad (1)$$

Vector $\mathbf{r}_{O_i}$ allows to describe the translation movements of the rigid body i , while the vectors $\mathbf{u}_i, \mathbf{v}_i, \mathbf{w}_i$ provide its orientation. Since the three unit vectors define a vector basis in space, it is possible to compute the kinematics of any generic point (P) or vector ($\mathbf{s}$) belonging to the body directly from its generalized coordinates using a set of transformation matrices, as presented below [29]

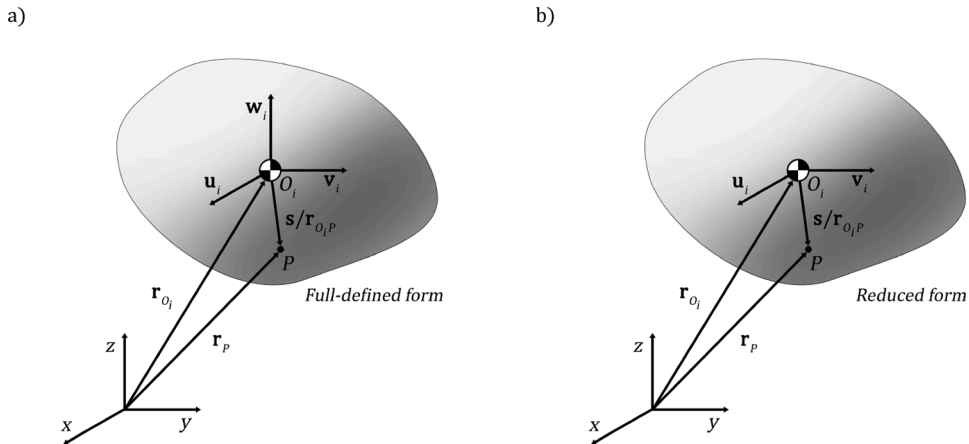


Fig. 1. Representation of the kinematic structure of a generic rigid body i with a generic point P and vector $\mathbf{s}$ belonging to it, modeled in its: a) fully-defined form; b) reduced form.

$$\mathbf{r}_P = \mathbf{C}_i^P \mathbf{q}_i \quad (2)$$

and

$$\mathbf{s} = \mathbf{C}_i^s \mathbf{q}_i \quad (3)$$

where $\mathbf{r}_P$ and $\mathbf{s}$ represent, respectively, the position vector for the generic point P and vector $\mathbf{s}$ in the global reference frame, and $\mathbf{C}_i^P$ and $\mathbf{C}_i^s$ the respective transformation matrices.

As it is possible to establish a vector basis using orthogonalization methods with two non-collinear vectors, the definition of the generic rigid body can be reduced to two unit vectors (see Fig. 1b)

$$\mathbf{q}_i = \{ \mathbf{r}_{O_i}^T \quad \mathbf{u}_i^T \quad \mathbf{v}_i^T \}^T \quad (4)$$

The reduced definition, given by Eq. (4), has the advantage of requiring less generalized coordinates and kinematic constraints than the fully-defined form, reducing the dimensions of the problem to solve. However, the definition of the kinematic constraints that describe the topology of the system requires the computation of the fully-defined equivalent vector ($\mathbf{q}_{3v_i}$) from the reduced form. This procedure is performed using a set of transformation matrices $\mathbf{S}$ and $\mathbf{V}$, which presents an explicit dependency on the generalized coordinates of the system, such as [29]

$$\mathbf{q}_{3v_i} = \mathbf{S} \mathbf{V}_i \mathbf{q}_i \quad (5)$$

with

$$\mathbf{S} = \begin{bmatrix} \mathbf{I}_3 & \mathbf{0}_3 & \mathbf{0}_3 & \mathbf{0}_3 \\ \mathbf{0}_3 & \mathbf{I}_3 & \mathbf{0}_3 & \mathbf{0}_3 \\ \mathbf{0}_3 & \mathbf{0}_3 & \mathbf{I}_3 & \mathbf{0}_3 \\ \mathbf{0}_3 & \mathbf{0}_3 & \mathbf{0}_3 & \frac{1}{2}\mathbf{I}_3 \end{bmatrix}_{(12 \times 12)} \quad (6)$$

and

$$\mathbf{V}_i = \begin{bmatrix} \mathbf{I}_3 & \mathbf{0}_3 & \mathbf{0}_3 \\ \mathbf{0}_3 & \mathbf{I}_3 & \mathbf{0}_3 \\ \mathbf{0}_3 & \mathbf{0}_3 & \mathbf{I}_3 \\ \mathbf{0}_3 & -\tilde{\mathbf{v}}_i & \tilde{\mathbf{u}}_i \end{bmatrix}_{(12 \times 9)} \quad (7)$$

This dependency implies that the degree of the kinematic constraints increases, and, consequently, the respective contributions to the Jacobian matrix (Φ_q). Moreover, the rigid body mass matrix becomes dependent on the generalized coordinates, also generating velocity-dependent inertial forces [29].

Thus, considering a mechanical model composed of nb bodies, the position and orientation of the multibody system is algebraically defined as

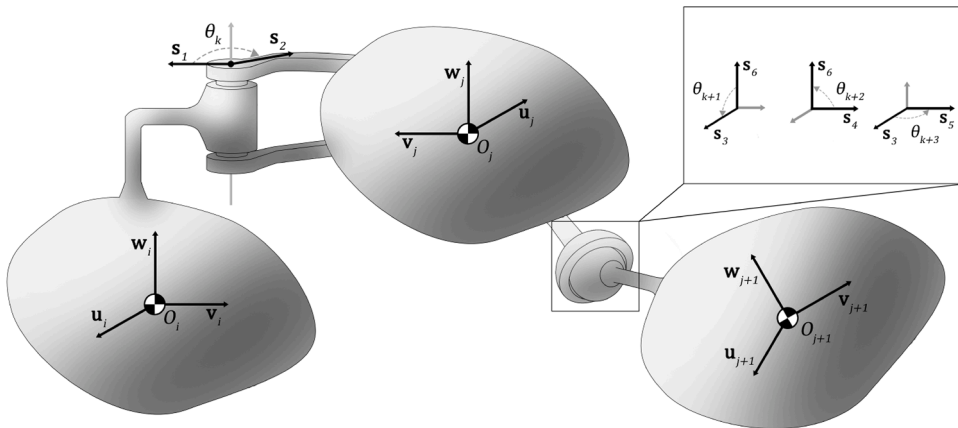


Fig. 2. Representation of the kinematic structure and the respective DoFs of a revolute joint defined between vector $\mathbf{s}_1$ of rigid body i and vector $\mathbf{s}_2$ of rigid body j and of a spherical joint defined between vectors $\mathbf{s}_3$ and $\mathbf{s}_4$ of rigid bodies j and vectors $\mathbf{s}_5$ and $\mathbf{s}_6$ of rigid body $j + 1$ modeled using an FCC-GRB formulation with MC.

$$\mathbf{q} = \{ \mathbf{q}_1^T \quad \dots \quad \mathbf{q}_i^T \quad \dots \quad \mathbf{q}_{nb}^T \}^T \quad (8)$$

where $\mathbf{q}$ is the vector of generalized coordinates of the entire system, including all the bodies defined in the fully-defined and reduced forms.

2.2. Mixed coordinates in an FCC-GRB formulation

When including an MC approach into the FCC-GRB formulation, the angular drivers (θ_k) that guide the model are also treated as generalized coordinates of the system to be solved (see Fig. 2). This approach has the advantage of allowing for the simultaneous computation of the coordinates and joint angles of the model that best fit the experimental data, without requiring a pre-processing step to calculate the drivers of the model. By minimizing the distance between the elements of the model and the equivalent elements of the experimental data, the method mitigates the effect of the experimental errors in the kinematic reconstruction of the movement, enabling to find the optimal model configuration that, on a given timestep, best-fits the experimental data.

Mathematically, the MC approach involves the addition of a set of angular variables (θ) to the vector of the generalized coordinates

$$\mathbf{q} = \{ \mathbf{q}_1^T \quad \dots \quad \mathbf{q}_i^T \quad \dots \quad \mathbf{q}_{nb}^T \quad \theta_1 \quad \dots \quad \theta_k \quad \dots \quad \theta_{nd} \}^T \quad (9)$$

where θ_k is the value of the angular displacement of the k -th driver of the model. Considering this approach, the number of angular variables to add should be equal to the number of DoFs to model using this approach (nd). It is worth mentioning that the total number of angular DoFs for the model can be higher, being the other DoFs guided using the traditional approach with kinematic constraint drivers as described in section 2.4.1.

The inclusion of the angular coordinates increases the total number of generalized coordinates of the system. Therefore, a set of angular-based constraint equations needs to be added to the vector of the kinematic constraints of the system (Φ) to express the topological dependencies between the FCC-GRB generalized coordinates and the angular coordinates (see Section 2.3). Moreover, additional linear tracking constraints need to be incorporated into the vector Φ to fit the model to the experimental data, effectively guiding the model throughout this process. It should be noted that, when analyzing (bio)mechanical systems, the reference data typically represent the position or orientation of relevant points or vectors in the model. Hence, two main types of tracking constraints are commonly used, namely the tracking constraint (TC) for guiding points and the tracking orientation constraint (TOC) for guiding vectors (see Section 2.4.2).

2.3. Kinematic constraints – Topologic definition

As it happens in other multibody formulations, the modeling of mechanical systems with FCC-GRB requires the mathematical definition of their topology. Gonçalves et al. presented a detailed description of the kinematic constraint equations needed for a comprehensive representation of a mechanical system in 3D, using the most common kinematic joints [29]. Consequently, the present work focuses only on the kinematic equations required to fully integrate the MC into the FCC-GRB formulation.

2.3.1. Mixed coordinates relation for a fully-defined body representation

From the topological point of view, the use of an MC approach requires the explicit definition of the geometric relations between the generalized coordinates of the FCC-GRB formulation and the newly introduced angular coordinates. This procedure can be described by one algebraic constraint equation that imposes a given angle between two unit vectors belonging to each of the bodies related by the DoF. Let one consider two generic unit vectors $\mathbf{s}_1$ and $\mathbf{s}_2$ belonging respectively to rigid bodies i and j (see Fig. 2), the mixed coordinates relation (MCR) is described in its homogenous form as

$$\Phi^{MCR}(\mathbf{q}_i, \mathbf{q}_j, \theta_k) = \mathbf{s}_1^T \mathbf{s}_2 - \cos \theta_k = 0 \quad (10)$$

where θ_k is the angular variable that describes the angular displacement between vectors $\mathbf{s}_1$ and $\mathbf{s}_2$ ($\theta_{s_1 s_2}$). By applying the linear transformation expressed in Eq. (3), the previous equation can be described in terms of the generalized coordinates of the system as

$$\begin{aligned} \Phi^{MCR}(\mathbf{q}_i, \mathbf{q}_j, \theta_k) &= (\mathbf{C}_i^{\mathbf{s}_1} \mathbf{q}_i)^T (\mathbf{C}_j^{\mathbf{s}_2} \mathbf{q}_j) - \cos \theta_k = 0 \\ \Phi^{MCR} &= \mathbf{q}_i^T \mathcal{C}^{\mathbf{s}_1 \mathbf{s}_2} \mathbf{q}_j - \cos \theta_k \end{aligned} \quad (11)$$

with

$$\mathcal{C}^{\mathbf{s}_1 \mathbf{s}_2} = \left[\mathbf{C}_i^{\mathbf{s}_1 T} \mathbf{C}_j^{\mathbf{s}_2} \right]_{(12 \times 12)} \quad (12)$$

Equation (11) expresses a quadratic relation between the generalized coordinates of bodies i and j . However, contrary to the premises of the FCC-GRB formulation, it also includes nonlinear terms that are dependent on the generalized angular variables. Therefore, the contributions to the Jacobian matrix (Φ_q), comprising the partial derivatives of the kinematic constraint equations with respect to the generalized coordinates of the system, include both the linear terms associated with the generalized coordinates of the two constrained bodies and an additional contribution associated with the angular variable θ_k , such that

$$\Phi_q^{MCR} = \left\{ \underbrace{\Phi_{q_i}^{MCR}}_{\mathbf{q}_j^T \mathcal{C}^{s_1 s_2} \mathbf{T}}, \underbrace{\Phi_{q_j}^{MCR}}_{\mathbf{q}_i^T \mathcal{C}^{s_1 s_2}}, \underbrace{\Phi_{\theta_k}^{MCR}}_{\sin \theta_k} \right\}_{(1 \times 25)} \quad (13)$$

Due to the constant nature of matrices $\mathbf{C}$, matrix $\mathcal{C}^{s_1 s_2}$ is also constant and time independent [29]. Moreover, the generalized angular variables do not present an explicit dependency on the time, indicating that Eq. (11) represents a scleronomic constraint. Thus, the contributions to the right-hand side vector of the velocities of the system (ν) are null

$$\nu^{MCR} = 0 \quad (14)$$

In turn, the quadratic and transcendental nature of the MCR condition implies that the contributions to the right-hand side vector of the accelerations (γ) include quadratic terms that depend on the generalized velocities of bodies i ($\dot{q}_i$) and j ($\dot{q}_j$), as well the generalized angular velocities ($\dot{\theta}_k$), such that

$$\gamma^{MCR} = -2\dot{q}_i^T \mathcal{C}^{s_1 s_2} \dot{q}_j - \dot{\theta}_k^2 \cos \theta_k = -2\dot{s}_1^T \dot{s}_2 - \dot{\theta}_k^2 \cos \theta_k \quad (15)$$

It should be noted that Eq. (11) represents one kinematic constraint equation that describes one rotational DoF associated with the kinematic joint defined by bodies i and j . Consequently, to fully describe the rotational DoFs associated with a specific kinematic joint, it is necessary to include, at least, one MCR constraint equation per DoF in the vector of the kinematic constraints, and the respective contributions to the Jacobian matrix and right-hand side vectors of velocity and acceleration.

Equations (13) to (15) can be simplified when the vectors that describe the MCR condition are directly rigid body vectors (e.g., $\mathbf{u}_i$ and $\mathbf{v}_j$). In this case, the definition of the MCR condition in its homogenous form is given by

$$\Phi^{MCR}(\mathbf{q}_i, \mathbf{q}_j, \theta_k) = \mathbf{u}_i^T \mathbf{v}_j - \cos \theta_k \quad (16)$$

This simplicity in the evaluation of the MCR kinematic constraint is also translated into the calculation of the respective contributions to Φ_q , ν and γ

$$\Phi_q^{MCR} = \left\{ \underbrace{\Phi_{u_i}^{MCR}}_{\mathbf{v}_j^T}, \underbrace{\Phi_{v_j}^{MCR}}_{\mathbf{u}_i^T}, \underbrace{\Phi_{\theta_k}^{MCR}}_{\sin \theta_k} \right\}_{(1 \times 25)} \quad (17)$$

$$\nu^{MCR} = 0 \quad (18)$$

$$\gamma^{MCR} = -2\dot{u}_i^T \dot{v}_j - \dot{\theta}_k^2 \cos \theta_k \quad (19)$$

2.3.2. Mixed coordinates relation for a reduced body representation

As previously mentioned, a reduced approach can be adopted to model the rigid bodies. In this case, the kinematic constraint equations needed to include the MC are similar to those used in the fully-defined case. However, the linear transformation presented in Eq. (5) should be applied to calculate the fully-defined equivalent vector, resulting in the following expression

$$\begin{aligned} \Phi^{MCR}(\mathbf{q}_i, \mathbf{q}_j, \theta_k) &= (\mathbf{C}_i^{s_1} \mathbf{S} \mathbf{V}_i \mathbf{q}_i)^T (\mathbf{C}_j^{s_2} \mathbf{S} \mathbf{V}_j \mathbf{q}_j) - \cos \theta_k = 0 \\ \Phi_q^{MCR} &= \mathbf{q}_i^T \mathbf{S} \mathbf{V}_i \mathcal{C}^{s_1 s_2} \mathbf{S} \mathbf{V}_j \mathbf{q}_j - \cos \theta_k \end{aligned} \quad (20)$$

The dependence of the matrices $\mathbf{V}$ on the generalized coordinates of the system implies an increase in the degree of the constraint equations. Nevertheless, as discussed in [29], the evaluation of the MCR constraint is highly efficient, as it only considers the algebraic multiplication of linear matrices and vectors dependent on the generalized coordinates of the system. This aspect is also valid for the contributions to the Jacobian matrix and right-hand side vector of accelerations

$$\Phi_q^{MCR} = \left\{ \underbrace{\Phi_{q_i}^{MCR}}_{\mathbf{q}_j^T \mathbf{V}_j^T \mathbf{S}^T \mathcal{C}^{s_1 s_2} \mathbf{T} \mathbf{V}_i}, \underbrace{\Phi_{q_j}^{MCR}}_{\mathbf{q}_i^T \mathbf{V}_i^T \mathbf{S}^T \mathcal{C}^{s_1 s_2} \mathbf{T} \mathbf{V}_j}, \underbrace{\Phi_{\theta_k}^{MCR}}_{\sin \theta_k} \right\}_{(1 \times 25)} \quad (21)$$

$$\begin{aligned} \gamma^{MCR} &= -\left(\mathbf{q}_i^T \mathbf{V}_i^T \mathbf{S}^T \mathcal{C}^{s_1 s_2} \dot{\mathbf{V}}_j \dot{\mathbf{q}}_j + \mathbf{q}_j^T \mathbf{V}_j^T \mathbf{S}^T \mathcal{C}^{s_1 s_2} \mathbf{T} \dot{\mathbf{V}}_i \dot{\mathbf{q}}_i + 2\dot{q}_i^T \mathbf{V}_i^T \mathcal{C}^{s_1 s_2} \mathbf{V}_j \dot{\mathbf{q}}_j \right) - \dot{\theta}_k^2 \cos \theta_k \\ \gamma^{MCR} &= -\left(\dot{s}_1^T \mathbf{C}_j^{s_2} \dot{\mathbf{V}}_j \dot{\mathbf{q}}_j + \dot{s}_2^T \mathbf{C}_i^{s_1} \dot{\mathbf{V}}_i \dot{\mathbf{q}}_i + 2\dot{s}_1^T \dot{s}_2 \right) - \dot{\theta}_k^2 \cos \theta_k \end{aligned} \quad (22)$$

where $\dot{\mathbf{V}}_i$ is the time derivative of the transformation matrix $\mathbf{V}$ for the body i defined following the methodology presented in [29]. Since Eq. (20) maintains its scleronomic nature, the contributions to the right-hand side vector of velocities for the reduced case remain null.

2.4. Kinematic constraints – Drivers definition

In addition to defining the topology of the system, the kinematic analysis of a multibody system requires the description of all the

DoFs associated with the mechanical model under analysis. Two main approaches can be considered to drive these DoFs, namely a methodology based on translational and angular drivers, or a method based on the minimization of a set of tracking constraints.

In the first approach, the angular DoFs need to be calculated from the experimental data, being subsequently fed in the system in the form of kinematic constraints of angular driver type that need to be satisfied for each time frame. The presence of artifacts in the experimental data will be reflected in the corresponding drivers, and, consequently, in the kinematic consistent positions computed during the analysis. A detailed description of the most common driver types used in FCC-GRB formulation can be found in [29].

The second method uses a set of tracking constraints and tracking orientation constraints, which express geometric relations between relevant points and vectors of the model and the respective experimental data, being minimized along the analysis. This method allows for an adaptation of the model to the prescribed data, mitigating the effect of possible experimental errors in the computation of the kinematic consistent positions. It is worth noting that other types of tracking constraints can also be incorporated. For example, the angular relation used to guide the model in the first method could be reformulated as a tracking constraint to be minimized. However, when applied to experimental data acquired using marker-based optoelectronic MOCAP systems, this strategy contrasts with the primary objective of automatically determining joint angular drivers that best reproduce the observed point positions, requiring also a pre-kinematic step to calculate the reference driver value. As this approach falls outside the scope of this study, it will not be explored. Nevertheless, in systems where only the positions of certain points and the joint angles are available, the method could be adapted to include such data, making it possible to compute a solution that fits both the point positions and minimizes the differences in angular drivers.

2.4.1. Angular drivers

Within the FCC-GRB formulation, the angular DoFs can be described using an AR condition. This kinematic constraint imposes that the relative angle between two vectors of the system is equal to a prescribed angle. Mathematically, the AR condition is similar to the formulation used to describe the MCR condition. However, it considers that the angular relation is made using the prescribed angle (θ_k^*) instead of the generalized angular variables (θ_k). Thus, let one consider two generic unit vectors $\mathbf{s}_1$ and $\mathbf{s}_2$ belonging respectively to rigid bodies i and j defined in their fully-defined form, the AR condition can be described in the homogenous form as

$$\Phi^{AR}(\mathbf{q}_i, \mathbf{q}_j, t) = \mathbf{s}_1^T \mathbf{s}_2 - \cos \theta_{s_1 s_2}^*(t) = (\mathbf{C}_i^{s_1} \mathbf{q}_i)^T (\mathbf{C}_j^{s_2} \mathbf{q}_j) - \cos \theta_{s_1 s_2}^*(t) = 0 \quad (23)$$

$$\Phi^{AR} = \mathbf{q}_i^T \mathcal{E}^{s_1 s_2} \mathbf{q}_j - \cos \theta_{s_1 s_2}^*(t)$$

where $\theta_{s_1 s_2}^*$ is the prescribed angle that describes the angular DoF between vectors $\mathbf{s}_1$ and $\mathbf{s}_2$ along the time. The AR condition expresses a quadratic relation between the generalized coordinates of the system, implying that their contributions to the Jacobian matrix are linear and equal to

$$\Phi_q^{AR} = \left\{ \underbrace{\mathbf{q}_j^T \mathcal{E}^{s_1 s_2}}_{\Phi_{q_i}^{AR}}, \underbrace{\mathbf{q}_i^T \mathcal{E}^{s_1 s_2}}_{\Phi_{q_j}^{AR}} \right\}_{(1 \times 24)} \quad (24)$$

Contrary to the MCR condition, the second term of Eq. (23) presents an explicit dependency on the time vector. Hence, the AR condition presents a rheonomic nature, meaning that the contributions to the right-hand-side vector of velocities and accelerations also include terms dependent on the time

$$\nu^{AR} = -\dot{\theta}_{s_1 s_2}^*(t) \sin \theta_{s_1 s_2}^*(t) \quad (25)$$

$$\gamma^{AR} = -2\dot{\mathbf{q}}_i^T \mathcal{E}^{s_1 s_2} \dot{\mathbf{q}}_j - \left(\left(\dot{\theta}_{s_1 s_2}^*(t) \right)^2 \cos \theta_{s_1 s_2}^*(t) + \ddot{\theta}_{s_1 s_2}^*(t) \sin \theta_{s_1 s_2}^*(t) \right) \quad (26)$$

Similarly to the MCR condition, Eq. (23) represents a single kinematic constraint that governs one DoF. Therefore, for each DoF of the model that is guided using an angular driver constraint, it is necessary to incorporate, at least, one AR condition into the vector of kinematic constraints.

When the vectors to constrain are rigid body vectors, Eqs. (23) to (26) can be simplified, obtaining

$$\Phi^{AR}(\mathbf{q}_i, \mathbf{q}_j, t) = \mathbf{u}_i^T \mathbf{v}_j - \cos \theta_{u_i v_j}^*(t) = 0 \quad (27)$$

For this case, the contributions to the Jacobian matrix and right-hand side vectors of velocities and accelerations are identical to those expressed by Eqs. (17) to (19), considering only the terms corresponding to the FCC-GRB generalized coordinates plus the rheonomic terms presented in Eqs. (25) and (26).

If a reduced rigid body definition is used for the definition of the model segments, the AR condition can be derived from Eq. (23), considering the computation of the fully-defined equivalent vector as presented in Eq. (5), yielding

$$\Phi^{AR}(\mathbf{q}_i, \mathbf{q}_j, t) = \mathbf{q}_i^T \mathbf{S} \mathbf{V}_i \mathcal{E}^{s_1 s_2} \mathbf{S} \mathbf{V}_j \mathbf{q}_j - \cos \theta_{u_i v_j}^*(t) = 0 \quad (28)$$

As for the fully-defined case, the definition of the AR condition in the reduced form is similar to the MCR condition (see Eq. (20)). However, the angular generalized coordinates are substituted by the prescribed angle. Therefore, the contributions to Φ , ν and γ are once again identical to those presented in Eqs. (21) to (22), considering only the terms corresponding to the generalized coordinates of

the system and the rheonomic terms expressed by Eqs. (25) and (26).

2.4.2. Tracking constraints

The formulation of the TC condition is similar to the linear translation driver described in [29]. However, instead of enforcing the distance between a model point and a reference point to be zero along the three axes of the global reference frame, it minimizes the distance between them. Let one consider a generic point P belonging to the rigid body i defined in its fully-defined form, the TC condition can be described in its homogenous form as

$$\Phi^{TC}(\mathbf{q}_i, t) = \mathbf{r}_{P_i} - \mathbf{r}_{P^*}(t) = \begin{Bmatrix} r_{P_{x_i}} - r_{P_x^*} \\ r_{P_{y_i}} - r_{P_y^*} \\ r_{P_{z_i}} - r_{P_z^*} \end{Bmatrix} = \mathbf{C}_i^P \mathbf{q}_i - \mathbf{r}_{P^*}(t) = \mathbf{0} \quad (29)$$

where $\mathbf{r}_{P^*}$ represents the prescribed coordinates of the reference point P^* in the global reference frame. Eq. (29) transforms into three linear constraint equations that guide three DoFs associated with point P , implying that the contributions to the Jacobian matrix are constant and equal to the corresponding matrix $\mathbf{C}$

$$\Phi_q^{TC} = \begin{bmatrix} \Phi_{q_i}^{TC} \\ \mathbf{C}_i^P \end{bmatrix} (3 \times 12) \quad (30)$$

It should be noted that the contributions can be assembled into the Jacobian matrix of the system during the kinematic pre-processing steps, eliminating the need for its update during the analysis and, consequently, reducing its computational effort. In turn, the rheonomic nature of the TC condition means that the contributions to the right-hand side vectors of the velocities and accelerations are not null, presenting explicit terms depending on the velocity ($\dot{\mathbf{r}}_{P^*}$) and acceleration ($\ddot{\mathbf{r}}_{P^*}$) of the reference point P^* , as presented below

$$\nu^{TC} = \dot{\mathbf{r}}_{P^*}(t) \quad (31)$$

$$\gamma^{TC} = \ddot{\mathbf{r}}_{P^*}(t) \quad (32)$$

In a similar way to the kinematic constraints, Eq. (29) can be adapted for the reduced definition of a rigid body using the linear transformation presented in Eq. (5). Thus, let one consider a reference point P^* belonging to a rigid body i defined in its reduced form, the TC condition and the corresponding contributions to Φ , ν and γ are given by

$$\Phi^{TC}(\mathbf{q}_i, t) = \mathbf{C}_i^P \mathbf{q}_{3v_i} - \mathbf{r}_{P^*}(t) = \mathbf{C}_i^P \mathbf{S} \mathbf{V}_i \mathbf{q}_i - \mathbf{r}_{P^*}(t) = \mathbf{0} \quad (33)$$

$$\Phi_q^{TC} = \begin{bmatrix} \Phi_{q_i}^{TC} \\ \mathbf{C}_i^P \mathbf{V}_i \end{bmatrix} (3 \times 9) \quad (34)$$

$$\nu^{TC} = \dot{\mathbf{r}}_{P^*}(t) \quad (35)$$

$$\gamma^{TC} = \ddot{\mathbf{r}}_{P^*}(t) - (\mathbf{C}_i^P \dot{\mathbf{V}}_i \mathbf{q}_i) \quad (36)$$

The use of the matrix $\mathbf{V}_i$ increases the degree of the kinematic constraint, implying that its contributions to the Jacobian matrix become dependent on the system generalized coordinates, and, consequently, it requires its update in each time step.

The tracking constraints can also be applied to map the orientation of a set of guiding vectors. In this case, the kinematic constraint equations in their homogeneous form are similar to those presented for a reference point P^* , considering the matrix $\mathbf{C}^s$ for a generic vector $\mathbf{s}$ (see Eq. (3)) instead of matrix $\mathbf{C}^P$. Therefore, let one consider a generic unit vector $\mathbf{s}$ belonging to rigid body i and the respective guiding vector $\mathbf{s}^*$, the tracking orientation constraint can be given by

$$\Phi^{TOC}(\mathbf{q}_i, t) = \mathbf{s}_i - \mathbf{s}^*(t) = \mathbf{C}_i^s \mathbf{q}_i - \mathbf{s}^*(t) = \mathbf{0} \quad (37)$$

or in the reduced form

$$\Phi^{TOC}(\mathbf{q}_i, t) = \mathbf{C}_i^s \mathbf{q}_{3v_i} - \mathbf{s}^*(t) = \mathbf{C}_i^s \mathbf{S} \mathbf{V}_i \mathbf{q}_i - \mathbf{s}^*(t) = \mathbf{0} \quad (38)$$

Mathematically, the TOC formulation is similar to the TC condition, which means that the contributions to the Jacobian matrix (Φ_q^{TOC}) are similar to those given by Eqs. (30) or (34), however, using the matrix $\mathbf{C}_i^s$. In turn, the contributions to the right-hand side vector of velocities (ν^{TOC}) and accelerations (γ^{TOC}) are equal to those expressed by Eqs. (31) and (32) or (35) and (36), considering the substitution of the transformation matrix $\mathbf{C}_i^P$ and the velocity and acceleration vectors of the reference point by the equivalent entities of vector $\mathbf{s}^*$, respectively $\dot{\mathbf{s}}^*$ and $\ddot{\mathbf{s}}^*$.

The TOC condition can also be applied to rigid body vectors. In this case, the kinematic constraint equation and the corresponding contributions to Φ simplify, becoming

$$\Phi^{TOC}(\mathbf{q}_i, t) = \mathbf{u}_i - \mathbf{s}^*(t) = \mathbf{0} \quad (39)$$

$$\Phi_{\mathbf{q}}^{TOC} = \begin{bmatrix} \Phi_{\mathbf{u}_i}^{TOC} \\ \mathbf{I}_3 \end{bmatrix}_{(3 \times 3)} \quad (40)$$

where $\mathbf{I}_3$ is the identity matrix. The contributions to the right-hand side vectors of velocities and accelerations are the same as the ones deduced for the fully-defined rigid body.

It is worth noting that each TOC condition guides two DoFs of the model, specifically the orientations around the two vectors orthogonal to the driven vector. As a result, the minimum number of TOC conditions required to ensure the proper fitting of the model to the reference data varies with the kinematic joint previously defined in the kinematic chain. For every revolute or universal joint of the model, at least one TOC condition guiding the child body needs to be added to the vector of the kinematic constraints of the system. Similarly, for driving rigid bodies constrained by spherical joints or guiding the orientation of a given rigid body with respect to the global reference frame, at least two TOC conditions are required to describe all three DoFs. To achieve a better fit between the model and experimental data, it is possible to add more TC and TOC conditions per segment. This procedure enables to find an optimal position that minimizes the distance to all the reference points and vectors, enhancing the accuracy of the analysis.

2.5. Kinematic analysis with mixed coordinates

The kinematic analysis allows for the determination of the kinematic positions of the model that comply with the imposed kinematic constraints and the prescribed drivers. Mathematically, it corresponds to the resolution of the kinematic constraint equations, defined in their homogenous form, with respect to the generalized coordinates of the system

$$\Phi(\mathbf{q}, t) = \{ \Phi_1^T \quad \dots \quad \Phi_i^T \quad \dots \quad \Phi_{nc}^T \}^T = \mathbf{0} \quad (41)$$

where Φ_i is the i -th set of kinematic constraint equations that define the mechanical system and nc denotes the total number of kinematic constraints. Given the non-linear nature of the kinematic constraints, Eq. (41) represents a set of nonlinear equations. Solving these equations, from a multibody framework, requires the use of proper methodologies to effectively obtain an accurate solution. Several methodologies can be employed to solve it, including numerical methods [17,24], optimization techniques [7,22], or artificial intelligence-based methods [37,38].

In the present work, three different approaches are compared to evaluate their influence on the solution accuracy and computational performance. The first method, the iterative Newton-Raphson method, is a well-established numerical approach that efficiently estimates the roots of a given function. The other two methods are based on optimization techniques, including a CNO with a weighted objective function and an MO goal attainment problem.

2.5.1. Newton-Raphson method

The iterative NRM is an efficient approach utilized to estimate the roots of a real function. Due to the nature of the numerical method that is in its origin, the NRM presents a quadratic convergence near the solution, meaning that, when the initial estimation is close to the solution, the method rapidly converges, allowing for the fast determination of the kinematic consistent positions for complex systems [39,40]. From a multibody point of view, the NRM can be formulated as [17]

$$\begin{cases} \Phi_{\mathbf{q}} \Delta \mathbf{q}_n = -\Phi(\mathbf{q}_n, t) \\ \mathbf{q}_{n+1} = \mathbf{q}_n + \Delta \mathbf{q}_n \end{cases} \quad (42)$$

where $\mathbf{q}_n$ and $\Delta \mathbf{q}_n$ are the solution and residuals of the NRM for the iteration n . For each time step, the iterative method presented in Eq. (42) is applied until the norm of the residuals vector is smaller than a tolerance established by the user ($\|\Delta \mathbf{q}_n\| < \epsilon$). The choice of the tolerance value determines the level of precision required for the solution, allowing the user to balance computational efficiency with accuracy.

Solving Eq. (42) requires that the lines of the Jacobian matrix are not linearly dependent or that the matrix is invertible. If the Jacobian matrix is singular or ill-conditioned, it suggests that there may be redundant or insufficient constraints in the system, leading to difficulties in finding a unique solution [41]. To fit the model to the experimental data, a set of kinematic drivers that need to be minimized is added to the kinematic constraints vector, usually in a number higher than the number of DoFs to guide, leading to the appearance of redundant constraints. In such cases, alternative methods must be considered to handle the non-invertibility of the Jacobian matrix. An efficient method considers the use of a least squares (LS) approach alongside the NRM, also referred to as Gauss-Newton algorithm, [42], which is formulated as

$$\Phi_{\mathbf{q}}^T \Phi_{\mathbf{q}} \Delta \mathbf{q}_n = -\Phi_{\mathbf{q}}^T \Phi(\mathbf{q}_n, t) \quad (43)$$

Besides allowing to handle a system defined with redundant constraints, this approach can be computationally preferable to Eq. (42), in most of the cases, as it generates symmetric equations that can be solved using efficient numerical methods based on pivoting

strategies [17].

The use of driving data contaminated with experimental errors can lead to the impossibility of finding a solution that satisfies all the constraint equations. In this case, the tracking constraint drivers, described in section 2.4.2, should not be treated as equations that must be strictly fulfilled, but rather as equations that need to be minimized throughout the analysis. This approach can be numerically achieved by allowing for the relaxation of these equations, using a weighted least squares method. Thus, Eq. (43) can be rewritten as

$$\Phi_q^T W \Phi_q \Delta q_n = -\Phi_q^T W \Phi(q_n, t) \quad (44)$$

with

$$W = \begin{bmatrix} w_1 & & & \\ & \ddots & & \\ & & w_i & \\ & & & \ddots \\ & & & & w_{nc} \end{bmatrix} \quad (45)$$

where W is the weight matrix, containing the weighting factors of each kinematic constraint (w_i). The use of the WLS-NMR has the advantage of solving the kinematic constraint equations without the need for complex optimization methods. However, the weights should be carefully defined to avoid the violation of the topological constraints, and, consequently, the determination of positions that are kinematically inconsistent. In particular, the weights associated with the topological constraints should be defined several orders of magnitude higher than those used to track the experimental data. This approach prioritizes enforcing the constraints that define the topology of the system over the driving constraints. Assigning higher weights to the topological constraints increases their influence on the solution, ensuring that the system follows the desired topological structure. On the other hand, the lower weights assigned to the tracking constraints provide flexibility in reaching those requirements.

2.5.2. Optimization

An alternative approach to perform the kinematic analysis of mechanical systems defined with tracking constraints is the use of optimization algorithms. In this case, the analysis is treated as an optimization problem, in which the topological kinematic constraint equations (Φ^{Top}) are defined as nonlinear equalities of the optimization and the tracking constraints as the objective function (F) that needs to be minimized. Hence, the optimization problem can be formulated as

$$\begin{aligned} &\text{Find : } \mathbf{q} \\ &\text{Minimize : } F(\mathbf{q}, t) \\ &\text{Subject to : } \begin{cases} \Phi^{Top}(\mathbf{q}, t) = 0 \\ \mathbf{q}_{lb} \leq \mathbf{q} \leq \mathbf{q}_{ub} \end{cases} \end{aligned} \quad (46)$$

where $\mathbf{q}_{lb}$ and $\mathbf{q}_{ub}$ are the vectors that contain the lower and upper bounds of the generalized coordinates, respectively. Considering a single-objective approach, the objective function can be defined as the weighted sum of the squares of the Euclidean distances (ED) between the coordinates of the model points ($\mathbf{r}_{p_n}$) and vectors ($\mathbf{s}_n$) and their corresponding positions in the experimental data ($\mathbf{r}_{p_n}^*$, $\mathbf{s}_n^*$)

$$F(\mathbf{q}, t) = \sum_{n=1}^{n_{TC}} w_n (\mathbf{r}_{p_n} - \mathbf{r}_{p_n}^*(t))^T (\mathbf{r}_{p_n} - \mathbf{r}_{p_n}^*(t)) + \sum_{n=1}^{n_{TOC}} w_n (\mathbf{s}_n - \mathbf{s}_n^*(t))^T (\mathbf{s}_n - \mathbf{s}_n^*(t)) \quad (47)$$

where w_n is the weighting coefficient of the n -th tracking equation, and n_{TC} and n_{TOC} are, respectively, the number of tracking constraints and tracking orientation constraints of the model. Considering the definition of a generic point in FCC-GRB, Eq. (47) can be rewritten as function of the generalized coordinates of the system as

$$F(\mathbf{q}, t) = \sum_{n=1}^{n_{TC}} w_n (\mathbf{C}_i^{p_n} \mathbf{q}_i - \mathbf{r}_{p_n}^*(t))^T (\mathbf{C}_i^{p_n} \mathbf{q}_i - \mathbf{r}_{p_n}^*(t)) + \sum_{n=1}^{n_{TOC}} w_n (\mathbf{C}_i^{s_n} \mathbf{q}_i - \mathbf{s}_n^*(t))^T (\mathbf{C}_i^{s_n} \mathbf{q}_i - \mathbf{s}_n^*(t)) \quad (48)$$

Equation (48) expresses a quadratic dependency of the objective function on the generalized coordinates of the system. This means that the gradient of the objective function $F(\mathbf{F}_q)$ can be easily determined, eliminating the need for methods relying on finite differences, which are traditionally slower. Accordingly, let one consider the n -th tracking equation, its contribution to $\mathbf{F}_q$ is given by

$$\mathbf{F}_q^{TCn}(\mathbf{q}, t) = 2(\mathbf{C}_i^{p_n} \mathbf{q}_i - \mathbf{r}_{p_n}^*(t))^T \mathbf{C}_i^{p_n} \quad (49)$$

Analogously, the contribution of the TOC condition to $\mathbf{F}_q$ is similar to the expression presented in Eq. (49), considering the substitution of the transformation matrix $\mathbf{C}$ associated with a generic point P by the transformation matrix corresponding to a generic vector $\mathbf{s}$, such that

$$\mathbf{F}_q^{TOCn}(\mathbf{q}, t) = 2(\mathbf{C}_i^{s_n} \mathbf{q}_i - \mathbf{s}_n^*(t))^T \mathbf{C}_i^{s_n} \quad (50)$$

In a similar manner to the NRM-WLS, the use of a weighted objective function enables tuning the model to relax the points that are less relevant to the system or more susceptible to experimental errors, improving the overall accuracy of the solution.

A different optimization approach, based on the use of a multi-objective goal attainment problem, can also be employed to perform the kinematic analysis of multibody systems, in which the contributions of each tracking constraint condition for the objective function are treated independently. Mathematically, the multi-objective goal attainment problem can be formulated as [43]

$$\begin{aligned} & \text{Find : } \mathbf{q} \\ & \text{Minimize : } Y \\ & \text{Subject to : } \begin{cases} \mathbf{F}(\mathbf{q}, t) - Y\mathbf{w}_{MO} \leq \mathbf{F}^*(\mathbf{q}, t) \\ \Phi^{Top}(\mathbf{q}, t) = \mathbf{0} \\ \mathbf{q}_{lb} \leq \mathbf{q} \leq \mathbf{q}_{ub} \end{cases} \end{aligned} \quad (51)$$

with

$$\mathbf{F} = \{ F^{TC_1} \quad \dots \quad F^{TC_n} \quad \dots \quad F^{TC_{n_{TC}}} \quad F^{TOC_1} \quad \dots \quad F^{TOC_n} \quad \dots \quad F^{TOC_{n_{TOC}}} \}^T \quad (52)$$

and

$$\mathbf{F} = \{ w^{TC_1} \quad \dots \quad w^{TC_n} \quad \dots \quad w^{TC_{n_{TC}}} \quad w^{TOC_1} \quad \dots \quad w^{TOC_n} \quad \dots \quad w^{TOC_{n_{TOC}}} \}^T \quad (52a)$$

where Y is the slack variable of the optimization defined as the maximum difference between the vector containing the objective functions ($\mathbf{F}$) and the goals of the optimization ($\mathbf{F}^*$) divided by the weight coefficients vector ($\mathbf{w}_{MO}$), which controls the relative degree of achievement of the goals.

In order to establish the individual cost function (F^{TC_n}), the ED condition between each reference point and its respective model point can be used, as presented in Eqs. (48) and (49). Consequently, each reference point contributes with one equation to the objective function vector. An alternative approach can be followed if, instead of using the ED, the TC condition is applied. In this case, the difference between the model and reference points is computed individually for each global direction, as detailed in section 2.4.2. Hence, each TC condition introduces three equations to the vector of the objective function, increasing the size of the problem to solve.

2.6. Dynamics analysis with mixed coordinates

The dynamic analysis of multibody systems defined with an FCC-GRB formulation and MC can be performed similarly to the classical FCC-GRB formulation. As the angular generalized coordinates are not used to define the rigid bodies, these can be removed from the vector of the generalized coordinates after the kinematic analysis has been performed. In the same way, the TC and TOC equations and the respective contributions to the Jacobian matrix and right-hand side vectors of velocities and acceleration should be discarded for the purpose of the dynamic analysis.

The elimination of the generalized angular variables entails the cancellation of terms associated with their partial derivatives from the Jacobian matrix. This procedure can be easily accomplished by directly deleting the columns of the Jacobian matrix that correspond to the angular variables. This approach is feasible because only the MCR kinematic constraints have an explicit dependency on the angular generalized coordinates. By removing the partial derivatives of θ , the contributions of the MCR condition become equal to the contributions of the AR condition. From a formulation perspective, implementing this procedure is equivalent to treating the angular generalized coordinates as drivers of the model. Therefore, the equations of motion (EoM) for an inverse dynamic analysis are given by

$$\mathbf{M}\ddot{\mathbf{q}} + \Phi_q^T \lambda = \mathbf{g} \quad (53)$$

where $\mathbf{M}$ represents the mass matrix of the system, $\mathbf{g}$ the vector of generalized forces and λ the vector of Lagrange multipliers. Moreover, the removal of the angular coordinates implies that the physical meaning of the Lagrange multipliers becomes equal to the ones obtained with a classical FCC-GRB formulation. Hence, the generalized internal forces associated with the MCR condition ($\mathbf{g}^{\Phi^{MCR}}$) become equal to the ones obtained with an AR driving constraint ($\mathbf{g}^{\Phi^{AR}}$), meaning that these represent a pair of symmetric concentrated moments applied in the two bodies constrained by this kinematic relation [29]. This fact implies that the joint moment of force associated with driver k (τ_k^{int}) can be computed as

$$\tau_k^{int}(t) = \lambda^{AR/MCR} \sin(\theta_{s_1 s_2}^*(t)) \mathbf{s}_{s_1 \perp s_2} \quad (54)$$

with

$$\theta_{s_1 s_2}^*(t) = \theta_k(t) \quad (55)$$

where $\mathbf{s}_1$ and $\mathbf{s}_2$ are the two generic vectors that define the MCR condition and $\mathbf{s}_{s_1 \perp s_2}$ a unitary vector normal to the plane defined by the two previous vectors. $\theta_{s_1 s_2}^*$ represents the angular driver for this condition, being equal to the corresponding angular variable computed

during the kinematic analysis with MC.

3. Implementation of the FCC-GRB formulation with MC

With the purpose of evaluating the effectiveness of the MC formulation within the context of a multibody formulation with fully Cartesian coordinates, the methodology presented in section 2 was implemented in an in-house multibody software, *H-Move*, developed in MATLAB language (The MathWorks Inc., Natick, MA) [29]. Furthermore, it was applied in the kinematic analysis of two mechanisms with different levels of complexity, namely a double-bar linkage (simple pendulum) with one DoF and a five-bar linkage constrained with spherical joints comprising a total of 12 DoFs (see Fig. 3). A detailed description of the multibody models, initial condition and experimental drivers are presented in Table A1 and A2 in Supplementary Materials (SM) A.

The accuracy and efficiency of the MC formulation with FCC-GRB were compared to the classical FCC-GRB formulation presented in [29]. For that purpose, the kinematic consistent positions of each point of the model were determined, considering a set of known drivers, by employing a kinematic analysis with NRM and an iteration tolerance of 10^{-10} . The duration of each simulation was set to 3 s considering a sampling frequency of 100 Hz. The angular drivers utilized for the reference data were generated using sinusoidal functions from known values (Amplitude: $\pi/6$ rad, Period: 3 s), and without any kind of noise.

In order to model experimental errors in the data, the kinematic consistent positions used as reference for the TC constraints were later perturbed by adding noise to the reference values previously calculated. For the simple model, white Gaussian noise was introduced to the experimental points with amplitudes of 7.5 mm and 30 mm in all directions. The first case corresponds to a maximum experimental error of 13 mm in relation to the reference point, an approximation of the values typically reported in the literature for the normal STA error. The second case considers a maximum displacement of 52 mm and represents an extreme case of STA [8,44,45].

For the complex model, instead of considering random white Gaussian noise, the input data were perturbed by introducing a sinusoidal wave in all directions, with a frequency within the range of typical human movement (3.3 Hz) and a maximum amplitude equal to that used in the simpler case, since this behavior better approximates the experimental error produced by the STA. To incorporate the error caused by electrical noise and marker vibration, white Gaussian noise with a maximum amplitude of 5 mm was posteriorly added to the experimental data. An example of the noise introduced in the reference data for the two models is shown in Figs. B.1 and B.2 of SM B.

Two test conditions were analyzed for the complex model. The first condition involved introducing perturbations to all model points and was used to evaluate the efficiency of different methods used to solve the kinematic equations and how effectively they fit the model points to the experimental data. In the second condition, the perturbations were applied only to points P_4 and P_9 and aimed at analyzing how the perturbations influence the propagation of errors along the kinematic chain and their impact on the angles computed using the MC approach. Additionally, a comparative analysis was conducted to evaluate the differences between using the MC approach and a traditional kinematic analysis with angular drivers computed from smoothed data. For this purpose, the kinematic data were filtered using a second-order zero-lag Butterworth filter with different cutoff frequencies: 9 Hz, 6 Hz, and 3 Hz. The choice of these values was based on the reference cutoff frequency of 6 Hz commonly used in gait analysis [46]. A stricter cutoff frequency (3 Hz), more suitable for slower movements, and a higher cutoff frequency (9 Hz), more appropriate for faster movements, were also considered.

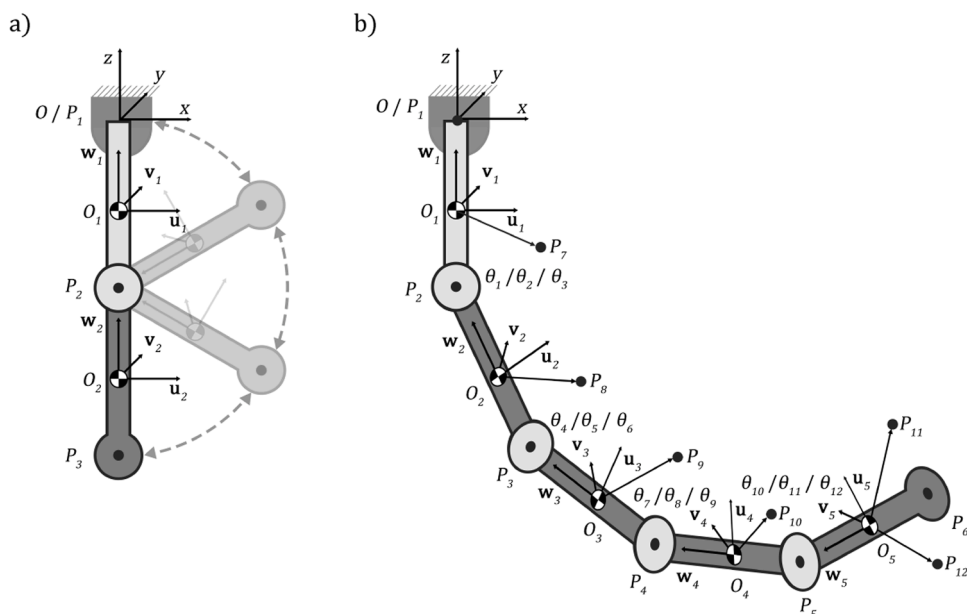


Fig. 3. Schematic representation of the two analyzed mechanisms: a) Double-bar linkage; b) Five-bar linkage.

To assess the computational differences between using different numerical approaches, each mechanism was evaluated using four different methodologies: a) NRM with LS; b) NRM with WLS; c) CNO with a single-objective weighted function; d) MO goal attainment problem. For condition a), no differences were considered between the topological kinematic constraints and the TC, i.e., it was assumed that all kinematic constraint equations have the same weight along the analysis. In condition b), the weights for the TC constraints were relaxed to 10^{-3} , while the topological constraints were maintained at 1. Finally, the same weight value of 1 was considered for each tracking condition of the cases c) and d). The differences between using an ED or a TC condition were also assessed for the MO optimization.

The kinematic analysis with NRM resorted to a set of custom-developed routines and considered an iteration tolerance of 10^{-6} and 10^{-10} . In its turn, the CNO with single-objective function and the MO attainment problem employed respectively the built-in functions *fmincon* and *fgoalattain*, available in the MATLAB optimization toolbox. A constraint tolerance of 10^{-10} was set for the optimization problems and the partial derivatives of the constraint equations and objective function were provided to the optimizer. For the CNO, two algorithms were analyzed, namely the interior-point and the sequential quadratic programming (SQP) method for the simpler model.

The accuracy of the analysis performed was determined by calculating the norm and the maximum value of the Euclidean distance vector between the position of each model point for the perturbed case and the reference data. Similarly, the norm of the vector containing the violations of the constraints that considers both all the kinematic constraint equations and only the topological conditions was computed to examine the effectiveness of the different methods in determining the kinematic consistent positions. For the evaluation of the computational efficiency, the time required to perform a kinematic analysis and the number of iterations per time step was evaluated. To understand the influence of using a different number of tracking points, the analysis of the five-bar linkage model also assessed the computational efficiency when using either eight or nine reference points to track the experimental data. Finally, the effect of using parallel computing to reduce optimization time was computed. In this case, the initial position was used as the initial guess for all the time frames.

The computational simulations were run on a single computer with the following specifications: CPU: Intel® Core™ i7-8700HQ, clocked at 3.2 to 4.6 GHz. For the trials with parallelization, a parallel pool of six workers was utilized. Each condition was tested 10 times consecutively to minimize the impact of computational performance fluctuations on the performance, with the computational times computed as the average time of all simulations.

4. Results

To begin with, it must be mentioned that no convergence issues were found for the different analyses conducted in this study. The four methods successfully allowed for the computation of a set of kinematic consistent positions that minimized the distance between the model points and the reference data. From an implementation point of view, incorporating the MC did not require significant changes to the theoretical structure underlying the FCC-GRB formulation. The methodologies described in sections 2.2 to 2.5 allowed for the modeling of the considered models, with their implementation being independent of the topology of the model. Furthermore, the methodology presented in section 2.6, which promotes the conversion of a system described with FCC-GRB with MC into a traditional FCC-GRB system, enabled the straightforward determination of the dynamic outcomes of the system, while preserving the same physical interpretation of the internal forces of the FCC-GRB formulation. Despite the success of the different approaches considered in this work to perform the kinematic analysis, these exhibited differences in terms of the accuracy of the solution and time required to reach it.

4.1. Double-bar linkage

4.1.1. Computational accuracy

The results obtained for all the conducted kinematic analyses closely matched the reference data, presenting an excellent agreement with the experimental inputs computed using known drivers (see Fig. 4 and Fig. C.1 in SM C). All methods accurately tracked the reference points, presenting errors lower than 10^{-5} m for the unperturbed case.

The outcomes show that the constraint violations over time are within the values specified for the method, except for the NRM method with LS (case a) and perturbed data (see Table 1). While this method was able to find a position that complies with the defined tolerances (10^{-10}), the analysis of the constraint violations for the topological constraints revealed higher-order values (maximum values of Φ_i^{top} of 3.5×10^{-12} for unperturbed case, 2.4×10^{-3} for a 7.5 mm perturbation and 8.9×10^{-3} for a 30.0 mm perturbation), suggesting the existence of inconsistencies in the definition of some topological constraints (e.g., shared point and vector constraints, ground relations). The analysis of the position and orientation of the model elements indicates that the model adjusted to the noisy tracking points, as it is shown in Fig. 4c. However, the minimization of the distance between the reference and simulation points was achieved by compromising the integrity of the kinematic joints. As a result, some of the points that should have remained fixed, according to the imposed constraints, changed their positions to better fit the model to the perturbed points.

The relaxation of the tracking constraints enabled to minimize this aspect. By decreasing the weights associated with the TC formulation, the magnitude of the violation of the topological constraints was greatly reduced, obtaining a maximum value on the order of 10^{-5} (maximum values of Φ of 2.4×10^{-12} for the unperturbed case, 1.2×10^{-5} for a 7.5 mm perturbation, and 5.7×10^{-5} for a 30 mm perturbation). In this case, the fixed points remained in their positions, with the displacement primarily occurring within the allowed DoF of the model.

Regarding the optimization-based methods, all of them successfully converged to an optimal solution that minimized the distance between the model points and the reference data, while maintaining kinematic consistency. The CNO achieved an average constraint violation per time step ranging between 10^{-11} and 10^{-10} . In turn, the MO goal attainment problem resulted in constraint violations of the same order, albeit with fewer iterations required per time frame. It is important to note that although negligible, the ED between the reference data and the optimization results for the case without perturbation was several orders of magnitude higher than the

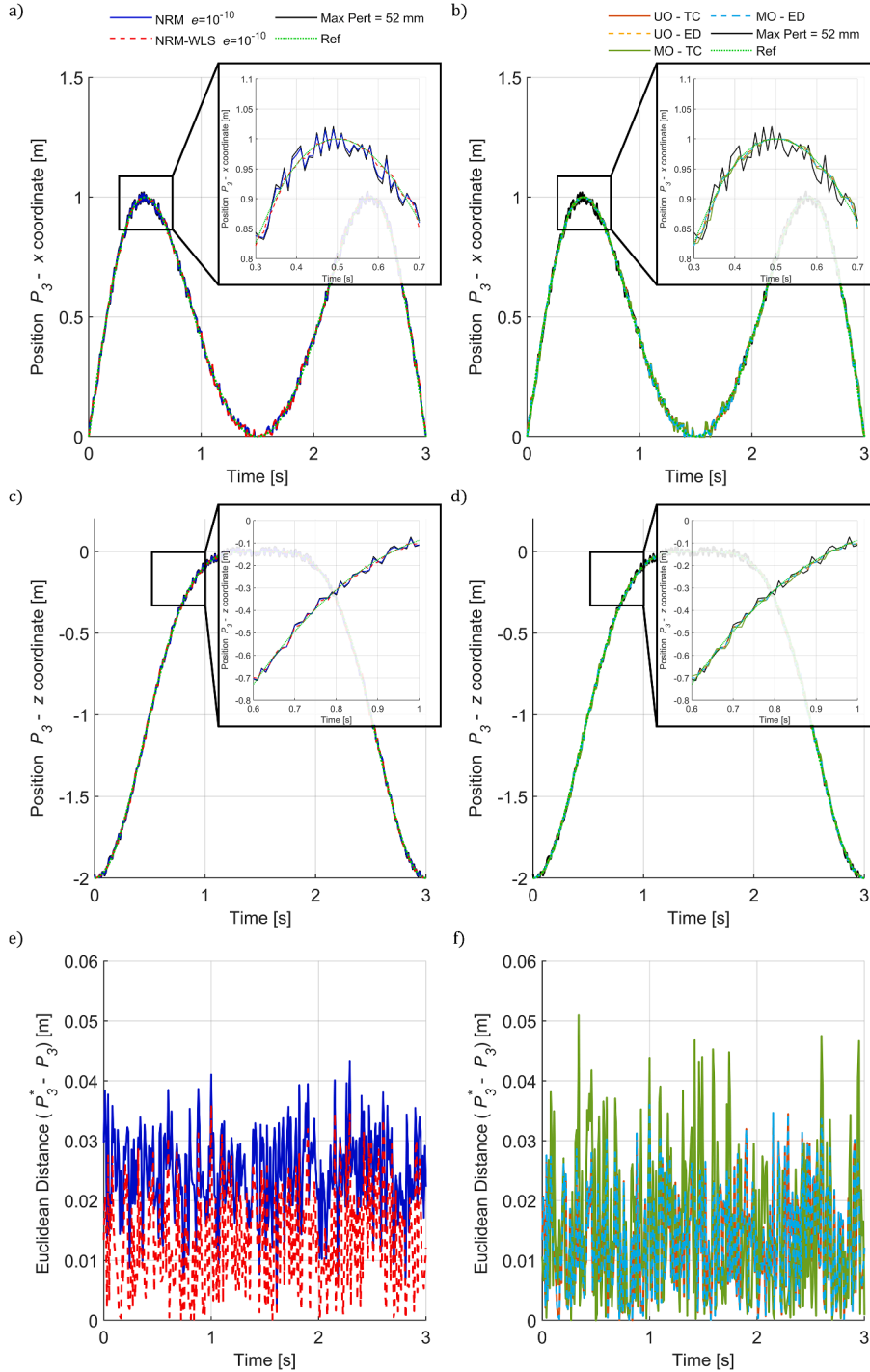


Fig. 4. Comparison between the KA results and reference data for P_3 of the double-bar linkage model with a maximum perturbation of 52 mm considering the NRM (left) and optimization algorithms (right): Top (a and b) – x coordinate; Middle (c and d) – z coordinate; Bottom (e and f) – Euclidean distance between the KA outcomes and reference data.

kinematic analysis with the NRM (see Figs. C.1 e-f in SM C), with the MO with TC presenting the higher values ($\sim 10^{-5}$ m) and the MO with ED with the lower ones (10^{-14} to 10^{-9} m). Regarding the CNO, no differences were observed between the TC or the ED constraint in the objective function, showing differences to the reference data in the order of 10^{-8} to 10^{-6} m.

4.1.2. Computational efficiency

To begin with, it must be said that all four methods converged quickly to the optimal solution, considering as an initial guess the position of the previous time frame. However, the number of iterations per time step and the computational time depended on the magnitude of the perturbation imposed on the reference data and the method used to perform the kinematic analysis (see Table 1).

As expected, the NRM method exhibited a lower number of iterations and faster convergence. In the absence of perturbations and considering a tolerance error of 10^{-10} , this method converged in approximately 2.6 s (8.6 ms/frame) for the simpler model, taking around 3 % more time than the kinematic analysis with AD. The increase of the iteration tolerance in four orders of magnitude resulted in a decrease of approximately 1 iteration per time frame and 21.8 % of the computational time. The inclusion of the perturbations in the TC drivers resulted in an increase of the computational time of 8.2 % (9.6 ms/frame) for the normal STA case and 51.7 % (13.5 ms/frame) for the extreme case.

The optimization-based methods for the unperturbed case required more time to find a solution than the NRM with WLS, ranging from 350 % (40.0 ms/frame) for the MO with ED objective function to 1928 % (170.0 ms/frame) in the case of the CNO with interior-point algorithm. The addition of the perturbations to the reference data resulted in a similar number of iterations per time frame and computational times of the unperturbed case. A significant difference in the computational performance was observed between the CNO with the default algorithm (interior-point method) and the MO attainment problem, with the latter taking approximately 78 % less time for the unperturbed case. The use of the SQP algorithm allowed to reduce significantly the optimization time for the CNO, reaching an average value of 42 ms/frame. An influence of the objective function can also be found in the MO optimization, with the ED-based function, which generates a lower number of objective functions, taking less time than the one based on the TC condition.

4.2. Five-bar linkage with perturbations in all reference points

4.2.1. Computational accuracy

The results obtained for the five-bar linkage with perturbations in all points were similar to those observed in the previous model (see Fig. 5 and Fig. C.2 in SM C). The NRM with LS and WLS allowed to achieve a solution that fulfils with the iteration tolerance defined for the analysis. For the unperturbed case, both methods achieved differences to the reference data in the order of 10^{-16} to 10^{-12} , while the optimization methods yielded values ranging from 10^{-8} and 10^{-4} . However, an adaptation of the generalized positions of the model points to the noisy reference points was observed when only the LS approach was utilized, leading to violations of the topological constraints (maximum values of Φ_i^{Top} of 3.9×10^{-3} for a 7.5 mm perturbation and 1.4×10^{-2} for a 30.0 mm perturbation). The relaxation of the TC weights allowed for the minimization of this issue, obtaining values in the order of 10^{-5} and 10^{-4} for the analyses with an iteration tolerance of 10^{-6} and 10^{-10} (see Table 2).

The optimization methods enabled the computation of a set of kinematic consistent positions that fit the reference data, while maintaining the maximum constraint violation under 10^{-10} . Although the different algorithms generated slightly different solutions, none directly followed the noisy data used as input. A significant difference in the kinematic patterns was observed between the results generated using parallel and sequential optimization, particularly for the perturbed cases. The inability to provide an initial guess near the solution for the parallel method resulted in a noisy pattern, as the method converged to similar positions that also fulfilled the topological constraints but did not necessarily represent the global minimum (see Fig. 5b and d). Moreover, some convergence problems were found in some time frames, even for the unperturbed case, leading to the appearance of some noisy artifacts in the results (see Table 2 and Fig. C.2 in SM C).

Table 1

Normalized computational time, average number of iterations per frame, mean constraint violations per frame and maximum value of the constraint violation for the topological kinematic constraints.

	<i>e</i>	Normalized Time [ms/frame]			N. Iterations			$\ \Phi\ $			Max Φ_i^{Top}		
		P0	P7.5	P30	P0	P7.5	P30	P0	P7.5	P30	P0	P7.5	P30
KA AD	10^{-6}	6.6	-	-	3.3	-	-	2.0×10^{-7}	-	-	7.9×10^{-7}	-	-
	10^{-10}	8.6	-	-	4.2	-	-	2.8×10^{-12}	-	-	2.7×10^{-11}	-	-
NRM LS	10^{-6}	7.0	7.4	9.1	3.0	3.3	4.1	1.1×10^{-7}	3.1×10^{-7}	2.3×10^{-7}	7.4×10^{-7}	2.4×10^{-3}	8.9×10^{-3}
	10^{-10}	8.9	11.1	13.5	4.0	5.0	6.3	9.9×10^{-13}	1.9×10^{-11}	2.5×10^{-11}	3.5×10^{-12}	2.4×10^{-3}	8.9×10^{-3}
NRM WLS	10^{-6}	6.9	7.5	9.0	3.0	3.3	4.0	1.1×10^{-7}	2.4×10^{-7}	2.4×10^{-7}	7.4×10^{-7}	1.2×10^{-5}	5.7×10^{-5}
	10^{-10}	8.8	9.6	13.5	4.0	4.9	6.5	1.0×10^{-12}	1.8×10^{-11}	2.4×10^{-11}	2.4×10^{-12}	1.2×10^{-5}	5.7×10^{-5}
CNO	IP 10^{-10}	171.4	173.1	179.2	24.0	24.1	24.3	5.0×10^{-11}	4.9×10^{-11}	5.2×10^{-11}	9.8×10^{-11}	9.9×10^{-11}	9.9×10^{-11}
	SQP 10^{-10}	42.3	42.1	43.0	3.3	3.3	3.4	1.1×10^{-12}	1.8×10^{-12}	4.3×10^{-12}	7.7×10^{-12}	3.6×10^{-11}	9.6×10^{-11}
MO	TC 10^{-10}	90.8	51.6	51.8	12.3	6.6	5.8	5.4×10^{-11}	9.1×10^{-12}	7.1×10^{-12}	9.9×10^{-11}	9.2×10^{-11}	9.9×10^{-11}
	ED 10^{-10}	40.0	41.0	43.3	4.9	5.0	5.1	5.4×10^{-12}	6.6×10^{-12}	9.6×10^{-12}	9.9×10^{-11}	9.6×10^{-11}	9.7×10^{-11}

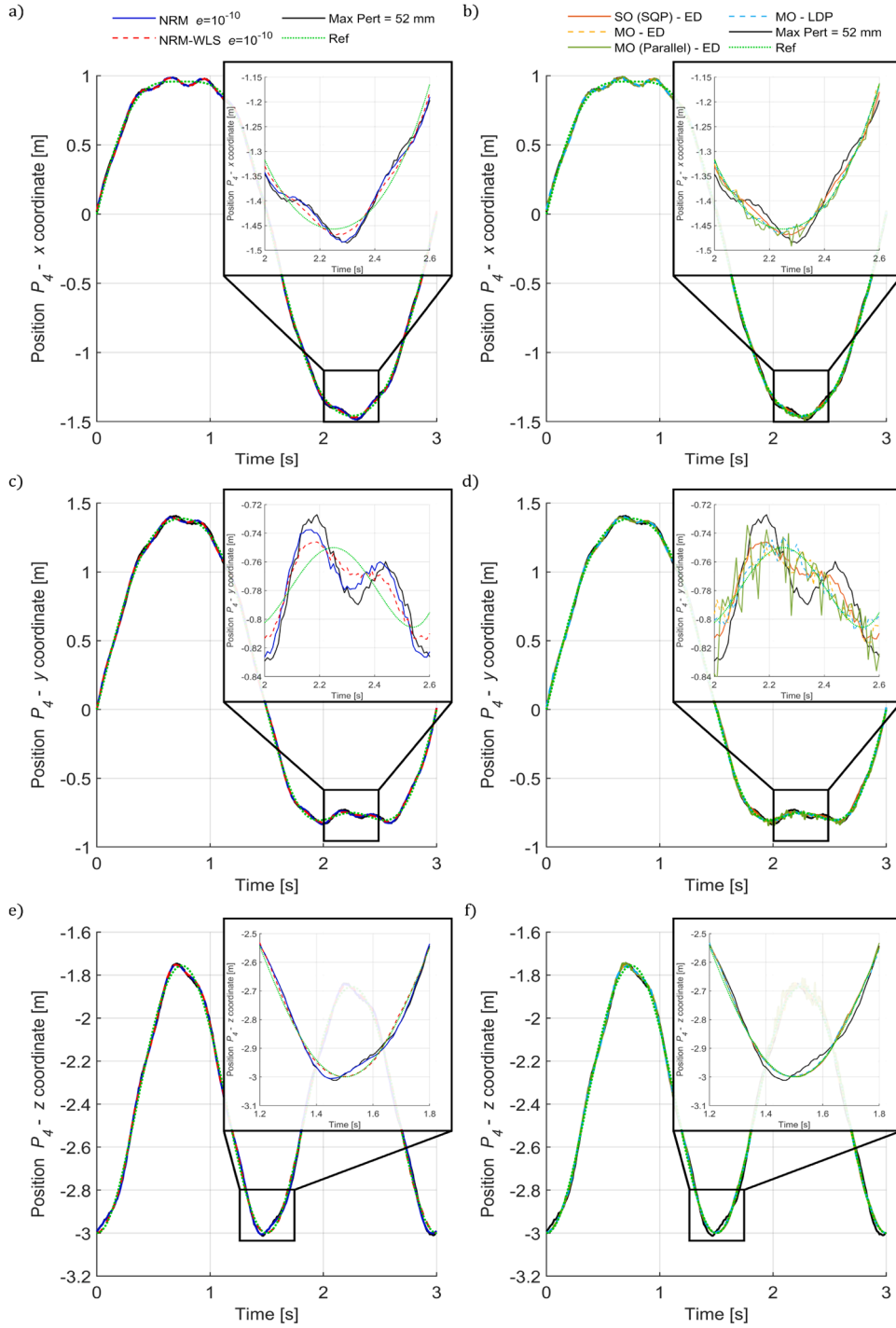


Fig. 5. Comparison between the KA results and reference data for P_4 of the five-bar linkage model with a maximum perturbation of 52 mm for all points considering the NRM (left) and optimization algorithms (right): Top (a and b) – x coordinate; Middle (c and d) – y coordinate; Bottom (e and f) – z coordinate.

Table 2

Normalized computational time, average number of iterations per frame, mean constraint violations per frame and maximum value of the constraint violation for the topological kinematic constraints.

	e	Normalized Time [ms/frame]			N. Iterations			$\ \Phi\ $			Max Φ_i^{Top}		
		P0	P7.5	P30	P0	P7.5	P30	P0	P7.5	P30	P0	P7.5	P30
KA AD	10^{-6}	16.2	-	-	3.6	-	-	8.2×10^{-8}	-	-	1.1×10^{-6}	-	-
	10^{-10}	18.4	-	-	4.0	-	-	6.6×10^{-12}	-	-	7.8×10^{-11}	-	-
NRM LS	10^{-6}	24.8	36.2	36.2	3.7	5.5	5.6	5.7×10^{-8}	3.2×10^{-7}	3.3×10^{-7}	1.1×10^{-6}	3.9×10^{-3}	1.4×10^{-2}
	10^{-10}	26.10	56.7	57.6	4.0	8.6	8.8	1.2×10^{-11}	3.4×10^{-11}	3.4×10^{-11}	4.3×10^{-11}	3.9×10^{-3}	1.4×10^{-2}
NRM WLS (8 ref pts)	10^{-6}	25.30	38.8	50.8	3.8	5.8	7.8	3.1×10^{-8}	3.4×10^{-7}	4.2×10^{-7}	9.8×10^{-7}	7.0×10^{-5}	2.5×10^{-4}
	10^{-10}	30.10	60.0	83.5	4.6	9.2	12.9	7.1×10^{-12}	3.1×10^{-11}	4.3×10^{-11}	1.1×10^{-10}	7.0×10^{-5}	2.5×10^{-4}
NRM WLS (9 ref pts)	10^{-6}	26.6	39.7	41.7	3.8	5.8	8.1	3.2×10^{-8}	3.4×10^{-7}	4.2×10^{-7}	9.0×10^{-7}	7.9×10^{-5}	2.8×10^{-4}
	10^{-10}	31.20	61.5	89.2	4.6	9.2	13.4	5.3×10^{-12}	3.5×10^{-11}	4.2×10^{-11}	1.6×10^{-10}	7.9×10^{-5}	2.8×10^{-4}
CNO (8 ref pts)	SQP	1199.2	1605.2	1384.7	34.1	46.7	48.1	1.2×10^{-15}	1.3×10^{-14}	2.4×10^{-13}	1.6×10^{-14}	3.8×10^{-13}	3.3×10^{-11}
	SQP Par	548.2	703.1	554.9	77.0	82.1	83.9	6.3×10^{-7}	4.7×10^{-6}	2.3×10^{-7}	1.9×10^{-4}	1.4×10^{-3}	8.8×10^{-11}
CNO (9 ref pts)	SQP	1420.3	1786.0	1848.6	38.1	45.9	46.9	1.6×10^{-15}	8.3×10^{-15}	1.1×10^{-14}	2.8×10^{-14}	3.5×10^{-13}	1.0×10^{-12}
	TC	1668.5	847.1	504.9	57.7	30.6	22.6	4.4×10^{-11}	1.4×10^{-11}	7.1×10^{-12}	9.9×10^{-11}	2.2×10^{-10}	9.6×10^{-11}
MO (8 ref pts)	ED	2120.7	1016.1	616.4	78.3	40.1	30.7	4.4×10^{-11}	2.6×10^{-11}	3.3×10^{-11}	1.0×10^{-10}	1.0×10^{-10}	1.0×10^{-10}
	TC Par	343.9	278.8	255.8	78.8	66.1	60.2	3.7×10^{-11}	1.3×10^{-11}	1.3×10^{-11}	1.0×10^{-10}	1.0×10^{-10}	9.9×10^{-11}
MO (9 ref pts)	ED Par	424.7	327.5	278.9	117.3	91.5	75.0	4.8×10^{-11}	2.3×10^{-11}	3.0×10^{-11}	9.9×10^{-11}	1.0×10^{-10}	1.0×10^{-10}
	TC	1748.5	847.4	683.1	56.7	28.4	23.0	4.5×10^{-11}	1.5×10^{-11}	9.9×10^{-12}	1.0×10^{-10}	1.0×10^{-10}	9.4×10^{-11}
	ED	2243.3	1150.1	884.1	76.5	40.6	32.1	4.7×10^{-11}	2.7×10^{-11}	3.1×10^{-11}	1.0×10^{-10}	1.0×10^{-10}	1.0×10^{-10}

4.2.2. Computational efficiency

The results for the more complex model with perturbations in all reference points show that the NRM is significantly faster than the best optimization case. Contrary to the simpler model, where the computational times were similar, the increase in model complexity resulted in a 57.7 % increase in computational time for the NRM with WLS with an iteration tolerance of 10^{-6} compared to the kinematic analysis with AD. This difference was significantly higher when the iteration tolerance was reduced to 10^{-10} , leading to an increase of 79.4 % in the average time per frame, even though an equivalent number of iterations per frame was observed.

For the unperturbed case, the CNO with SQP was faster than the MO with both TC and ED objective functions. This trend reverted when the perturbations were added to the input data, with the MO with TC function converging faster. This inversion can be understood by the lower number of iterations and function evaluations that this method requires to converge. Moreover, with the increase of the perturbation, the normalized time per frame reduced for the MO cases.

The use of a parallelization strategy with six pools resulted in a reduction of the computational cost, ranging from five times faster in the unperturbed case to two times in the maximum perturbation case. The lower efficiency of parallelization for the more perturbed cases can be explained by the reduction of the relative difference in the number of iterations required to find a solution between the sequential and parallelization cases. In contrast, the reduction for the CNO was approximately two times for all cases.

In general, using one additional tracking point led to an increase in computational cost. This difference was more visible in the optimization analyses, with increases ranging from 3.0×10^{-2} % for the MO with TC and lower perturbation to 43.4 % for the MO with ED and higher perturbation. The results for the NRM with WLS and an iteration tolerance of 10^{-10} showed increases ranging from 2.5 % to 6.8 %.

4.3. Five-Bar linkage with perturbation on P_4 and P_9

To simulate the effect of STA in markers more prone to this artifact and evaluate its influence on the propagation of errors along the kinematic chain, a third condition, where only P_4 and P_9 were perturbed, was tested, revealing significant differences between methods (see Fig. 6 and Fig. C.3 in SM C). The results suggest that both the NRM-WLS and the optimization methods can correct the perturbations introduced earlier in the kinematic chain. The positions achieved for the last point of the open chain closely matched the reference position. In contrast, the kinematic analysis with AD and perturbed drivers exhibited substantial discrepancies in terms of the kinematic patterns, reflecting the noise introduced in the data. This difference is clearly evident in the Euclidean distance plot, which showed a maximum distance of 0.05 m for the smaller perturbed case and 0.21 m for the maximum perturbed case. The results indicate that the NRM with WLS tends to generate smaller differences compared to the optimization methods; however, it comes at the cost of not ensuring such strict compliance of the kinematic constraints.

Fig. 7 presents one of the joint angular drivers computed for P_4 using the MC approach. The results show that even when introducing perturbations in the point that defines this joint and the nearest one P_9 , which assists in tracking the segment longitudinal rotations, the method can compute a consistent angle that matches the reference driver, while reducing the noise. For the normal STA values, the angle pattern follows the reference without significant oscillations (see Fig. 7a). On the other hand, for the maximum perturbed case, although the computed angle follows the expected trend, it still exhibits oscillations throughout the analysis, which are more noticeable in the MO-ED case (see Fig. 7b). It is worth mentioning that the magnitude of these oscillations is significantly lower than what is observed when the drivers are computed from the perturbed data.

The comparison between the MC approach and the use of smoothed noisy angular drivers is presented in Fig. 8. The results show that the MC method using NRM-WLS leads to position and velocity profiles closer to the reference data than any of the smoothed driver

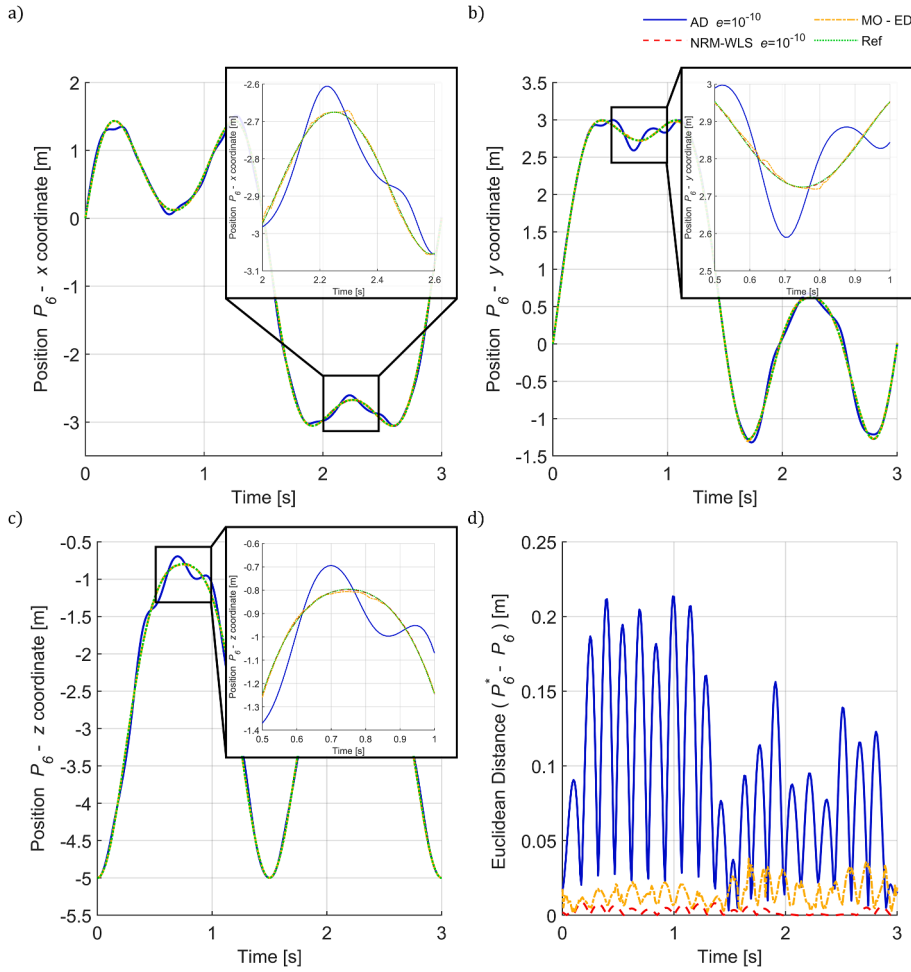


Fig. 6. Comparison between the KA results and reference data for P_6 of the five-bar linkage model with a maximum perturbation of 52 mm in P_4 and P_9 considering the AD with perturbed drivers, NRM-WLS and MO with ED: a) x coordinate; b) y coordinate; c) z coordinate; d) Euclidean distance between the KA outcome and reference data.

cases (see Fig. 8a-b), as well as to lower Euclidean distances (see Fig. 8c). Although smoothing the experimental data reduces the influence of the perturbed data on the kinematic results, the Euclidean distances remain approximately one order of magnitude higher than those obtained with the MC approach. For the reference cutoff frequency of 6 Hz, commonly adopted in gait analysis, the average reduction in distance was approximately 21.7 % (see Fig. 8c). Applying a stricter cutoff frequency further reduced both the Euclidean distance and the magnitude of the high-frequency oscillations observed in the joint driver signals (−34.9 %), approximating also the velocity curves of the reference data. However, it should be noted that cutoff values around 3 Hz may be overly restrictive, potentially attenuating meaningful motion components of the signal and thereby compromising the accuracy of both kinematic and dynamic outcomes [46].

The results obtained with the 3 Hz filter further emphasize the advantages of the MC approach over angular-based driving methods, particularly in minimizing the propagation of artifacts along the kinematic chain. Despite reducing noise levels in the joint angles to values similar to those achieved by the MC method (see Fig. 8d), the magnitude of the differences in the point positions remained higher (see Fig. 8c). This outcome stems from the absence of a global fitting process in the angular-based driving methods, implying that perturbations introduced in earlier segments of the chain are directly propagated throughout the system. Furthermore, it should be highlighted that fitting the model to the experimental data enhances not only positional accuracy but also the accuracy of velocity and acceleration patterns, ultimately improving the quality of the dynamic outcomes.

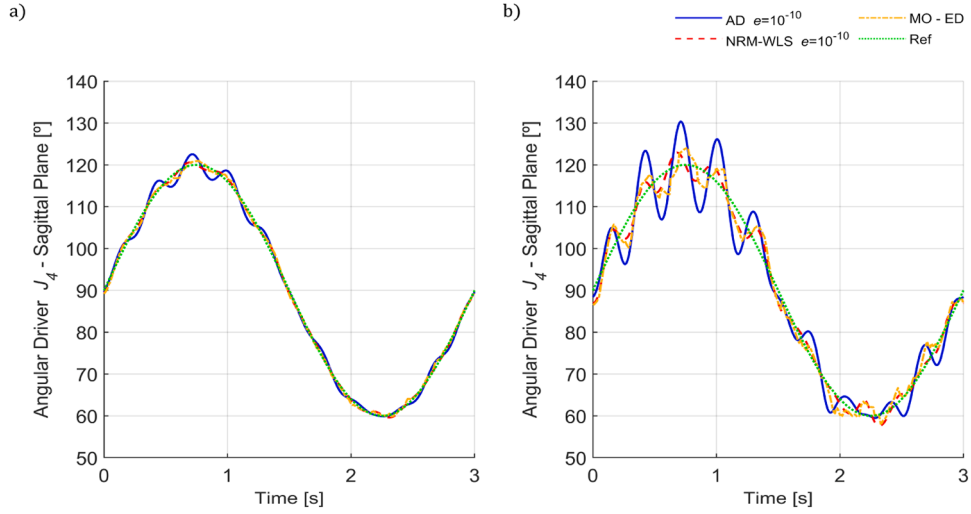


Fig. 7. Comparison between the joint angular driver computed using MC and reference data for point P_4 in the five-bar linkage model with NRM-WLS and MO-ED: a) maximum perturbation of 13 mm in P_4 and P_9 ; b) maximum perturbation of 52 mm in P_4 and P_9 .

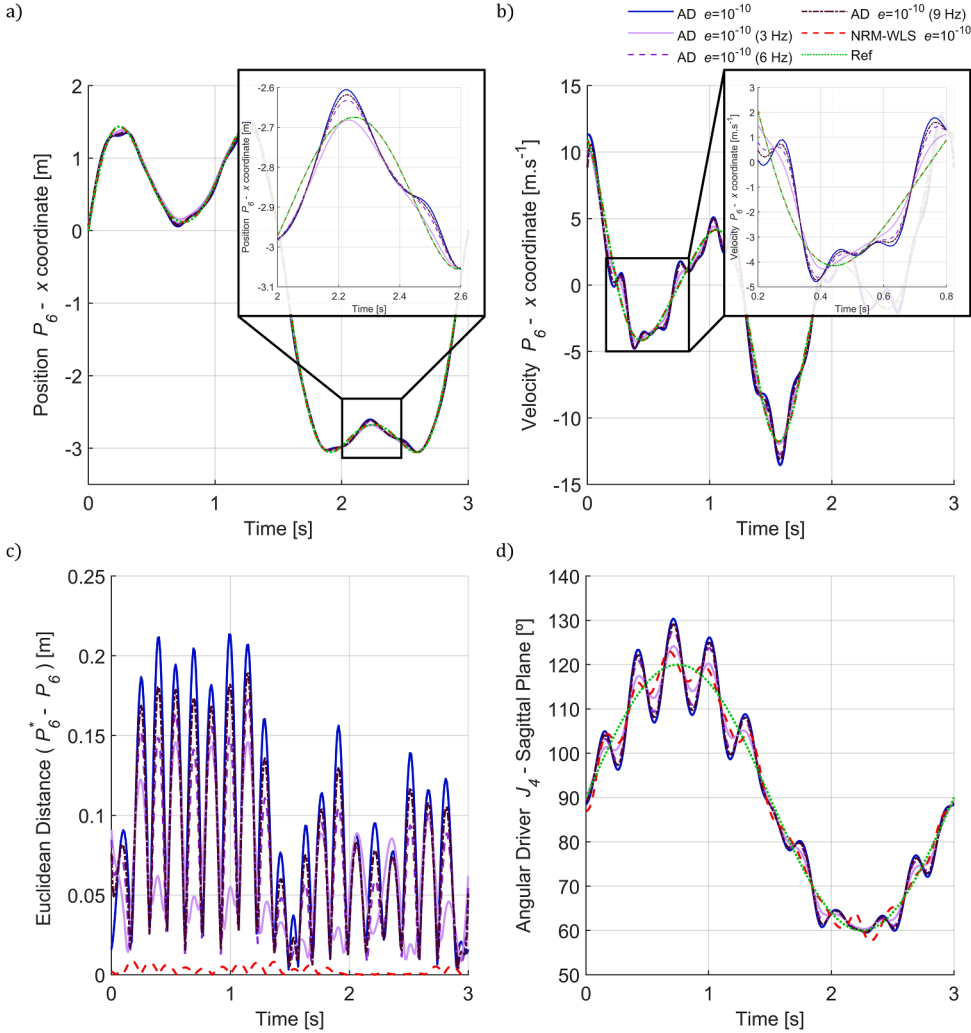


Fig. 8. Comparison between the KA results and reference data of the five-bar linkage model with a maximum perturbation of 52 mm in P_4 and P_9 considering the AD with perturbed drivers with and without filtering, and NRM-WLS: a) x coordinate of point P_6 ; b) x velocity of point P_6 ; c) Euclidean distance between the KA outcome and reference data for point P_6 ; d) Joint angular driver for point P_4 .

5. Discussion

The present study expands the fully Cartesian formulation with a generic rigid body to encompass the inverse kinematic and dynamic analysis of multibody systems with Mixed Coordinates and evaluates the accuracy and efficiency of different methods. The adoption of an MC formulation enables the computation of the kinematically consistent positions of the model that better fit the reference data, while simultaneously calculates the angular drivers of the model, which describe the DoFs associated with the kinematic joints. This modeling approach enables the evaluation of the major kinematic outcomes in a single analysis, eliminating the need for additional steps to compute the drivers of the model.

Besides simplifying the modeling procedure and pre- and post-kinematic steps, the presented approach also offers advantages related to the accuracy of the solution. By minimizing the distance between the tracking markers and the corresponding points of the model, the method determines a kinematically consistent position that accurately represents the overall position of the model in relation to the experimental data. This methodology addresses the issues commonly associated with the use of angular drivers, namely the propagation of errors along the kinematic chain due to the computation of drivers from noisy or inconsistent data. Moreover, the use of different weights can force the model to follow points that are less prone to experimental errors or are more relevant to the analysis. It should be noted that this study specifically focused on open-chain models, where error propagation is typically more pronounced due to the absence of topological constraints to enforce positional consistency along the chain. Nonetheless, since the MC method with FCC-GRB maintains the same principles of the global FCC-GRB formulation, it does not face the limitations commonly associated with recursive formulations in the analysis of closed-loop systems [29,47], and, consequently, it can be applied to analyze such systems without requiring significant modifications.

From the implementation point of view, incorporating the angular coordinates into the formulation is a straightforward process. The angular DoFs of the system, which are traditionally modeled using angular drivers, are here treated as angular variables that are evaluated during the process of computing the kinematically consistent positions. The AR kinematic constraints, which describe the angular relation between two vectors of the model, are replaced by an MCR condition. In fact, the two conditions are similar, being the rheonomic term of the AR constraint equations substituted by a similar term dependent on the generalized coordinates of the system. This relation implies that the inverse dynamic analysis of a system defined using MC is also a straightforward process. The simplicity of this procedure is related to the fact that one system modeled with MC and FCC-GRB can be easily converted to a classical FCC-GRB model, by transforming the angular generalized variables into angular drivers and by removing the tracking constraints. Therefore, the physical meaning of the internal forces computed using the Lagrange method is the same, not requiring additional steps besides the ones already performed in the classical formulation. It is worth mentioning that although this work details the implementation of a spatial MC formulation based on FCC-GRB, this approach can be applied in other global formulations, considering the specific characteristics of each formulation [17,34,35]. Moreover, transitioning to a 2D FCC-GRB formulation can be easily performed by applying the same concepts as those employed in the spatial formulation, but using the equivalent planar expressions [28]. In this particular case, the key difference lies in the lower minimum number of tracking constraint equations needed to fully describe the system kinematics, as the rigid bodies and kinematic joints have fewer DoFs.

The results obtained for the two analyzed models support the previously mentioned advantages. Both the NRM and optimization methods were able to find a kinematically consistent solution, while simultaneously determining the angular drivers of the model. The NRM method was significantly faster than the different optimization conditions tested in this work. This result is a direct consequence of the nature of the NRM algorithm, which exhibits a quadratic convergence near the solution [39,40]. This fact implies that if an initial guess near the solution is given to the iteration algorithm, it will converge quickly to the solution. The use of the NRM method to solve kinematic equations is not without limitations. The classical problems typically associated with the NRM algorithm can occur, including convergence issues when initiating with a poor initial guess or one far from the solution, overshoot effects due to the bad behavior of the function near the solution, or null-derivative functions [39,40,48].

Regarding the optimization methods, the MO attainment goal proved to be the faster solution for the more complex model. The results indicate an influence of the type of objective function utilized. Despite generating more equations than the ED condition, the use of the TC-based objective function resulted in lower computational times for the more complex model, a difference in part explained by the lower number of iterations required to find a solution. This trend was not observed in the simpler model, indicating that the relative differences in the computational times may be strongly affected by the complexity of the model under analysis and the optimization inputs. In fact, the simulations for the cases with higher levels of perturbation converged faster than the ones with lower levels, requiring also less iterations to find an optimal solution. In contrast, the CNO with SQP converged significantly faster than with the IP algorithm. Conversely to the MO case, the increase in the perturbation levels resulted in higher computational times and a higher number of iterations to find a solution. It should be noted that the gradients of the equality constraint equations and objective functions were provided to the optimizer. The use of finite differences significantly increased the simulation time; however, this difference was not quantified in this analysis.

In general, the incorporation of the angular coordinates led to an increase in the computational effort for all conditions when compared to the classical FCC-GRB formulation with angular drivers. Nevertheless, it is worth noting that the pre- and post-processing steps required for computing the drivers are not included in the analysis, and no fitting to the reference data is performed. In contrast, in the MC analyses, both the computation of the generalized coordinates and the angular drivers are carried out simultaneously and are accounted in the computational costs.

In terms of accuracy, the kinematic analyses with the NRM method did not yield results as exact as those obtained with the optimization methods. Since the TC and TOC kinematic equations are treated as equality constraints that must be fulfilled, the method generates kinematic positions that, in order to adapt the model to the noisy reference points, may violate some of the constraints. The

use of different weights for the topological and tracking constraints enables the mitigation of this difficulty. By relaxing the weights associated with the tracking constraints, the method assigns less significance to these equations, prioritizing the fulfillment of the topological constraints. This idea is supported by the results obtained for the analyses with perturbations. The maximum value of the topological constraints violation during the analysis decreased by two orders of magnitude when a weight of 10^{-3} was used. This difference can be even increased if lower weights are assigned to the TC equations, or higher weights are given to the topological constraints. This better fitting to the experimental points is also supported by the lower ED to the reference points. Overall, the NRM method presented lower values than the optimization-based methods. This difference is particularly noticeable in the cases without perturbations, meaning that the NRM can be the preferable choice in terms of accuracy when the input data does not present noise or artifacts.

One of the advantages of using optimization methods is the treatment of the tracking constraint equations as objective functions to be minimized during the dynamic analysis. This approach ensures that only the topological constraints are treated as equality constraints, thus preventing violations of these constraints. All the sequential optimizations resulted in maximum constraint violations for the topological constraints on the order of 10^{-10} and 10^{-11} , within the number of iterations and function evaluation defined for the analysis and considering a constraint tolerance of 10^{-10} . It should be noted that for some positions of the five-bar linkage model, the CNO with the interior-point algorithm presented convergence problems due to the system matrix becoming close to singular or badly scaled, reaching the maximum number of iterations.

Despite reducing the average time of the analysis, the use of a parallel approach to solve the optimization problem resulted in a noisy pattern. This outcome can be explained by using the initial position as the optimization initial guess for all time frames. The method converged for similar positions that comply with the optimization equality constraints, but do not represent the global minimal point. Hence, the kinematic positions should be post-processed to avoid unrealistic accelerations, as these could impact the dynamic outcomes. An alternative solution to mitigate this issue is to first perform an analysis using the NRM and WLS and then use the results from this analysis as initial guesses for the optimization problem. Another approach is to subdivide the entire problem into as many sub-problems as the available threads, solving the kinematic analysis sequentially within each sub-problem. However, while this strategy addresses the issue of noisy positions within each sub-problem, it may introduce the challenge of ensuring data continuity at the boundaries between sub-problems.

Hence, considering the advantages and limitations of the tested methods, optimization algorithms should be the preferred choice when analysis accuracy is critical, while the NRM with WLS should be employed when computation effort is an important factor, or the input data does not present noise or perturbations.

It is worth mentioning that a 3-second analysis period sampled at 100 Hz was used in this study, as this duration exceeds the typical cycle times observed in human motion. For example, a full gait cycle at normal cadence lasts approximately 1.1 s [49–51]. While this duration might be considered short for simulation-based analyses [52], the present study focuses exclusively on the inverse dynamic analysis of (bio)mechanical systems, which does not require integration steps. Therefore, as long as the initial guess for each time frame is close to the actual solution, both the numerical and optimization-based methods are expected to converge without numerical problems. In the approach adopted here, the output from one time frame serves as the initial guess for the subsequent frame, further ensuring proximity to the solution and promoting fast convergence. This assumption may not hold for very fast motions; however, in such cases, an increased acquisition frequency is typically required to accurately capture the dynamics of the movement [53], thereby mitigating this issue.

A relevant feature of the MC formulation with FCC-GRB is that it largely preserves the principles of the classical FCC-GRB approach. Therefore, the advantages reported for the classical formulation are still maintained. However, the inclusion of angular coordinates in the vector of the generalized coordinates implies that the system is no longer exclusively defined using Cartesian coordinates. Consequently, kinematic constraint equations incorporating nonlinear terms dependent on angular variables are generated. Since these variables do not directly define the rigid bodies, they do not impact the definition of the rigid body topological constraints or the computation of other points or vectors of the model, as the definition of the transformation matrices $\mathbf{C}$ and $\mathbf{V}$ remains equal. Therefore, most of the kinematic constraints maintain their linear or quadratic nature, meaning that their contributions to the Jacobian matrix and right-hand side vectors of velocities and accelerations are still null, linear or quadratic with respect to the generalized coordinates. This independence of the rigid bodies' definition from the angular generalized variables implies that the definition of the system mass matrices is the same as in the classical formulation, considering the elimination method described in section 2.6.

Although forward dynamics is not the primary focus of this hybrid formulation or of the analyses presented in this study, the MC formulation with the FCC-GRB framework has the potential to be adapted for the forward dynamics analysis of mechanical systems. While the increased dimensionality of the system is expected to raise computational demands, no additional numerical challenges are anticipated beyond those commonly encountered in traditional FCC-GRB simulations, such as singular configurations, redundant constraints, ill-conditioned Jacobian and mass matrices, or integration stability problems [29,41,54]. Future work also aims to explore extending the MC with FCC-GRB to incorporate flexible bodies or adopting alternative solving strategies based on different optimization algorithms or artificial intelligence approaches [37,38,55–58].

The similarities between the classical FCC-GRB formulation and the FCC-GRB with MC in terms of implementation and modeling procedure imply that the straightforwardness associated with the classical approach remains applicable in the second case. The potential applications identified for the classical formulation, such as teaching multibody dynamic topics in higher education, are still valid [28,29]. Although the MC variation includes angular variables, it does not require a high level of expertise in 3D rotation parametrization. This characteristic aligns with the advantages often highlighted when utilizing the natural coordinates formulation in advanced educational contexts [35].

The intrinsic properties of the FCC-GRB formulation also make it particularly suitable for the biomechanics of motion field. Since

the points and vectors that compose the generic rigid body have a direct relation with the inertial information found in anthropometrical databases, the modeling process becomes straightforward. The incorporation of the MC simplifies the inverse dynamic analysis of biomechanical models, as the reference points and vectors can be defined in the measure that they directly represent the markers used in the experimental acquisition of movement. Moreover, the rigid body vectors can be easily aligned with the anatomical joint axes, directly defining the rotation directions. If the generalized angular drivers are defined to match the convention established for the joint angles ([3,4]), the methodology can directly provide the joint angles.

Finally, as highlighted in the introduction, experimental data acquired using traditional marker-based optoelectronic motion capture systems are prone to STA, which, due to their frequency characteristics and unpredictable nature, are difficult to automatically detect and attenuate using conventional smoothing techniques. By fitting the biomechanical multibody model, typically defined using measurements taken during static acquisitions with the markers placed at the correct anatomical landmarks, the MC helps mitigate STA effects, thereby improving both kinematic and dynamic analyses. This advantage is particularly significant, as both dynamic and muscle analysis outcomes are highly sensitive to perturbations in kinematic data [15,59,60]. Hence, in addition to simplifying the pre- and post-processing steps, the MC method enhances the accuracy of kinematic data, ultimately improving the reliability of biomechanical analysis.

It is also important to mention that the use of the MC approach increases the complexity of the system, particularly when solved from a forward dynamics perspective, due to the increase in the number of coordinates and kinematic constraint equations. When applied in an inverse kinematic context, the increase of the system complexity has less impact on the computational performance of the analysis, making it more suitable for this type of study. In fact, the kinematic analysis with NRM and WLS for the five-bar linkage took approximately 30 ms per frame to converge, indicating its potential for real-time applications. This time could be improved by using a reduced definition of the model or by using a faster compiled programming language instead of an interpreted one. In certain scenarios, employing an MC formulation can offer additional modeling advantages when applied from a forward dynamics or predictive standpoint [35]. The explicit use of angular variables can simplify the control of specific systems that rely on angular inputs and facilitate the modeling of the action of external torque actuators, such as passive and active exoskeletons and wheelchairs [61–65].

6. Conclusions

This work explores the use of an MC formulation with FCC-GRB in the inverse kinematic and dynamic analysis of spatial multibody systems. The major steps required to fully implement the formulation, both with fully-defined and reduced rigid bodies, are described in detail. The formulation is validated in the analysis of two models with different levels of complexity. The accuracy and computational differences between using a numerical method based on the NRM and optimization algorithms are analyzed to evaluate the applicability of the formulation within different contexts. The results indicate that in terms of accuracy, optimization-based methods ensure the kinematic consistency of the system, albeit the increase in computational effort. The use of an NRM with WLS allows for the reduction of the computational cost, as it enables to control the violation of constraints at a topological level by defining appropriate weights.

From an implementation point of view, the use of an MC formulation with FCC-GRB offers the main advantage of simultaneously computing the kinematically consistent position and drivers associated with the joint angular DoFs. This procedure is achieved by treating the joint displacement angles as generalized coordinates of the system and by minimizing the distance between a set of points and vectors of the model and their respective reference data. As a result, there is no need for pre- or post-processing steps to obtain all kinematic outcomes, avoiding also the errors associated with the use of angular drivers, such as the propagation of experimental errors along the kinematic chain.

Despite requiring the explicit use of angular variables, the adoption of MC does not require complex parametrizations of 3D angle rotations, maintaining the simplicity of implementation typically attributed to the natural coordinates and classical FCC-GRB formulation. Therefore, it is the authors' belief that this formulation remains suitable not only for teaching multibody-related topics but also for other areas that require kinematic analyses of complex systems with noisy experimental data, such as biomechanics of movement.

CRedit authorship contribution statement

Sérgio B. Gonçalves: Writing – review & editing, Writing – original draft, Validation, Software, Methodology, Investigation, Formal analysis, Conceptualization. **Ivo Roupa:** Writing – review & editing, Validation, Conceptualization. **Paulo Flores:** Writing – review & editing, Supervision. **Miguel Tavares da Silva:** Writing – review & editing, Supervision, Project administration, Conceptualization.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

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Supplementary materials

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Data availability

No data was used for the research described in the article.

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