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Fully analytical sensitivity analysis of flexible multibody systems in natural coordinates

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In this work, a fully analytical formulation for the sensitivity analysis of flexible multibody systems in natural coordinates is derived, extending the analytical sensitivity formulations for rigid bodies, already available in the bibliography.

For the representation of the flexibility, the floating frame of reference (FFR) method is used. The flexible approach intends to be general, within the framework of FFR, and therefore no assumptions on the floating frame or on the deformation modes are adopted and a continuum mechanics approach based on invariant shape integrals is adopted for the inertia terms coming from the flexible bodies.

The implementation of the sensitivity equations was coded in MBSLIM, an in house library for the dynamics and sensitivity analysis of multibody systems. The general implementation aimed, exposed the limitations of the natural coordinates formulations published in the bibliography, which lacked the generality required here, motivating the thorough derivation accomplished here, not only for sensitivities but also for the dynamics equations of motion in natural coordinates.

For simplicity, this work focuses only on the natural coordinates ALI3-P equations of motion with direct sensitivities, but the library features also adjoint sensitivities and many other formulations in natural coordinates and recursive formulations in

joint coordinates. For this reason, the multidimensional matrix algebra (which might seem unnecessary complex at first) is in the core of the equations and it is crucial for simplifying expressions and for keeping a minimal number of terms and sharing code between very different formulations, which make use of the same exact pieces but arranged differently in direct sensitivities vs. adjoint and/or between different sets of equations of motion.

1 Introduction

Slender structures and flexible mechanisms are steadily gaining presence in many fields of industrial design, specially in robotics, aeronautics and in the automotive industry. Flexible Multibody Systems (FMBS) represent a formalism for modeling these kind of systems in which deformation is not negligible. In past decades, the challenge was the accurate and efficient dynamic analysis of these mechanisms [1, 2, 3], but lately more researchers have been focusing on their optimal design and performance optimization. Sensitivity analysis is an indispensable tool in local gradient-based optimization and a very valuable tool in mechanical design and optimization of multibody systems as well, being this need early identified in [4].

Several techniques have been proposed over the years to convert the infinite number of degrees of freedom (DoF) of a flexible body to a finite number, being the finite element methods (FEM) the most widely used. Methods based on FEM employ a set of global coordinates which describe the total displacement of each node (and eventually some additional DoF), resulting in a large number of coordinates and an intense computational effort for the methods based on this approach.

Model order reduction methods (MOR) emerged as a means of reducing the computational burden while keeping the necessary information to capture the fundamental deformation of the flexible bodies. The basis of the methods and a description of the most typical deformation modes is described in [5].

The Floating Frame of Reference method (FFR) [1], exploits the MOR theory for the representation of the flexible deformation. The motion of a flexible body is decomposed in small deformations superposed to the rigid body motion by the Rayleigh-Ritz method. The method is widely used in flexible multibody dynamics because of its versatility and low computational effort.

One of the most complex aspects of the FFR formulation is the derivation of the mass matrices for the inertia terms. A continuum mechanics approach based on invariant shape integrals is used in this work for efficiently building the flexible mass matrices, similar to those presented in [1, 6] but particularized for natural coordinates and with important theoretical and implementation simplifications because of the multidimensional algebra used.

The shape integrals approach is more complex than those proposed in [7, 8] based on a projection of the FEM mass matrix onto the rigid-flexible multibody coordinates but it is also more general because it does not rely on the properties of the lumped mass or consistent FEM mass matrices for an efficient evaluation of the multibody flexible mass matrices. Trying to avoiding shape integrals can be a good choice if third party FEM software is employed and only dynamics is needed but, in the case of this

work, analytical sensitivity analysis is pursued, forcing to evaluate additional integrals not provided for third party codes.

Recently, several works have proved the growing interest of the multibody community in the sensitivity analysis of flexible multibody systems based on the FFR approach. Gufler et al. presented in [9] analytical expressions for the FFR formulation based on the lumped mass approach and point of reference coordinates [10].

MBSLIM [11], is a library for the dynamics and sensitivity analysis of multibody systems. It was developed, in origin, for the dynamic simulation of rigid multibody systems in natural coordinates and it was later endowed with sensitivity analysis capabilities and more recently extended with topological formulations in joint coordinates. In this work, the extension to accommodate flexible bodies in the dynamics and direct sensitivity with the ALI3-P global formulation in natural coordinates is covered.

The ALI3-P target formulation described in this work is thoroughly described in [12] for rigid bodies, while its direct and adjoint sensitivity analysis was covered in [13, 14]. The extension of a natural-coordinates rigid body FFR formulation to flexible was already accomplished in [15] but with some limitations: 1) the actual description is more general than the previous ones, because of the requirement of implementing it in a general purpose library; 2) a tangent frame was employed before in order to simplify the description, while here a Bucken's [16, 17, 18] type floating frame is chosen for generality; 3) for versatility, no simplifications concerning the type of deformation modes are being adopted when building the dynamic terms, which makes it possible the combination of modes of different natures, like free dynamic modes, constrained dynamic modes, static modes, constraint modes, or impact modes, among others.

The multidimensional matrix algebra is ubiquitous in the equations presented in this work, which can be seen as an unnecessary level of complexity but there is a good reason for adopting the approach: the whole extension of MBSLIM will be not only for the formulation and sensitivity approach mentioned here but also for the adjoint sensitivity approach described in [14, 19], for other global formulations like the ones described in [20, 21] and even for other recursive formulations in joint coordinates described in [22, 23, 24]. It happens that most of the formulations make use of the same dynamic terms and derivatives, but arranged in a different way. The same applies to direct vs. adjoint sensitivities: they make use of the same pieces as part of totally different equations. Having those minimal pieces separately and being able of combining them with different magnitudes by tensor algebra, leads to a minimal code which can be shared between different formulations and sensitivity approaches, leading to an easier maintenance.

Although the main contribution of this work is on the sensitivities side, the kinematic description presented in this work for natural coordinates is novel. In the process of overcoming the limitations for extending MBSLIM, the kinematic description in natural coordinates had to be reformulated, arriving at a unified description for points and unit vectors in the rigid body part and a flexible body description which includes rigid body kinematics as a particular case.

The work is structured as follows: section 2 covers the kinematic description of a flexible body; section 3 presents the dynamic equations of the FFR method in natural coordinates, including the assembly of the mass matrix and internal and external

forces; in section 4, the sensitivity analysis of the dynamic equations of section 3 is described along with the required derivatives of masses, forces and constraints; in section 5 both dynamic and sensitivity equations are tested in two numerical examples; finally, section 6 presents the conclusions of the work. The document is completed with two appendices: appendix A, on multidimensional matrix algebra and appendix B, covering the detailed derivation of mass matrices shape integrals. The reading of appendix A on high-order matrix algebra is advised for a better understanding of the notation used in this document.

2 Kinematic description of a flexible body

According to Fig. 1, the position of a point P in body i expressed in the local reference frame of the body, can be divided in rigid body and flexible contributions:

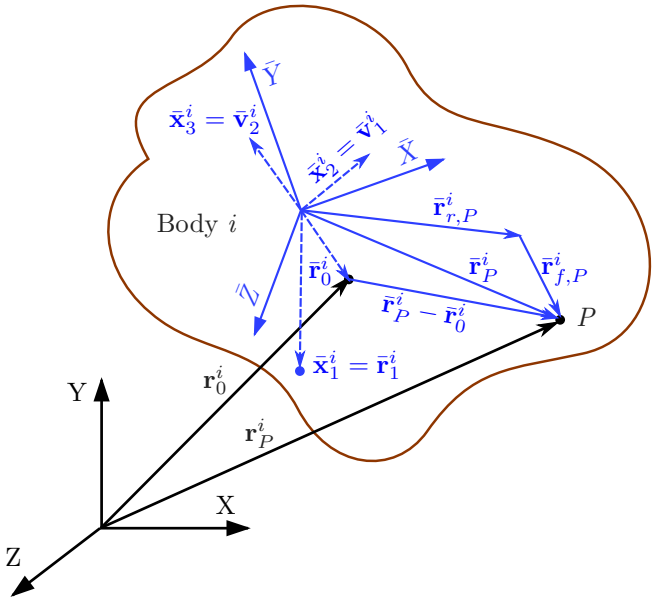


Fig. 1: Kinematic description of a flexible body in natural coordinates: the floating frame rigid-body modeling entities are represented in dashed line (in this particular case, two points $\bar{\mathbf{r}}_0^i$, $\bar{\mathbf{r}}_1^i$ and two vectors $\bar{\mathbf{v}}_1^i$, $\bar{\mathbf{v}}_2^i$). Local coordinates are represented in blue.

$$\bar{\mathbf{r}}_P^i = \bar{\mathbf{r}}_{r,P}^i + \bar{\mathbf{r}}_{f,P}^i \tag{1}$$

$$\bar{\mathbf{r}}_{f,P}^i = \bar{\boldsymbol{\varphi}}_P^i \mathbf{q}_f^i \tag{2}$$

The upper bar means local coordinates, the rigid body contribution, $\bar{\mathbf{r}}^i_{r,P}$, is the vector of local coordinates in the undeformed configuration (which is constant), $\bar{\mathbf{r}}^i_{f,P}$ is the deformation expressed in the local frame, which can be written as a linear combination of the deformation modes in the point, $\bar{\boldsymbol{\varphi}}^i_P \in \mathbb{R}^{3\times n^i_f}$ with the flexible coordinates $\mathbf{q}^i_f \in \mathbb{R}^{n^i_f}$ as coefficients.

The position of the point in the global reference frame:

$$\mathbf{r}^i_P = \mathbf{r}^i_0 + \mathbf{A}_i\left(\bar{\mathbf{r}}^i_P - \bar{\mathbf{r}}^i_0\right) = \mathbf{r}^i_0 + \mathbf{A}_i\left(\bar{\mathbf{r}}^i_{r,P} + \bar{\mathbf{r}}^i_{f,P} - \bar{\mathbf{r}}^i_0\right) = \mathbf{r}^i_{r,P} + \mathbf{r}^i_{f,P} \tag{3}$$

where $\mathbf{r}^i_0$ is the position, expressed in the global frame, of a reference point, rigidly attached to the body i local frame; $\mathbf{A}_i \in \mathbb{R}^{3\times 3}$ is the rotation matrix of the body, $\mathbf{r}^i_{r,P} = \mathbf{r}^i_0 + \mathbf{A}_i\left(\bar{\mathbf{r}}^i_{r,P} - \bar{\mathbf{r}}^i_0\right)$ is the rigid body part, i.e., the undeformed position of the point in the global frame and $\mathbf{r}^i_{f,P} = \mathbf{A}_i\bar{\mathbf{r}}^i_{f,P}$ accounts for the flexible deformation.

In natural coordinates, using rotation matrices for expressing positions of rigid body points or vectors is unusual and linear combinations of the rigid body modeling points/vectors are used instead:

$$\mathbf{r}^i_P = \mathbf{r}^i_{r,P} + \mathbf{r}^i_{f,P} = \bar{\mathbf{C}}^i_P\mathbf{q}^i_r + \mathbf{A}_i\bar{\mathbf{r}}^i_{f,P} = \mathbf{D}^i_P\mathbf{q}^i \tag{4}$$

where $\mathbf{q}^i_r = \left[\mathbf{r}^{i\mathrm{T}}_0\ \mathbf{x}^{i\mathrm{T}}_1\ \mathbf{x}^{i\mathrm{T}}_2\ \mathbf{x}^{i\mathrm{T}}_3\right]^{\mathrm{T}} \in \mathbb{R}^{12}$ are the rigid body natural coordinates modeling the body i floating frame (see Fig. 1), being $\mathbf{x}^i_1$, $\mathbf{x}^i_2$, $\mathbf{x}^i_3$ points or unit vectors, $\mathbf{q}^i = \left[\mathbf{q}^{i\mathrm{T}}_r\ \mathbf{q}^{i\mathrm{T}}_f\right]^{\mathrm{T}} \in \mathbb{R}^{n^i}$, with $n^i = 12 + n^i_f$, is the full set of rigid and flexible modeling coordinates of the body, $\mathbf{D}^i_P = \left[\bar{\mathbf{C}}_P\ \mathbf{A}_i\bar{\boldsymbol{\varphi}}^i_P\right] \in \mathbb{R}^{3\times n^i}$ the full matrix of linear combination with $\bar{\mathbf{C}}^i_P \in \mathbb{R}^{3\times 12}$ constant and $\bar{\mathbf{C}}^i_P\mathbf{q}^i_r$ accounting for the rigid body motion.

Because the rotation matrix in natural coordinates only depends on the rigid body coordinates of the body, the following linear relation can be deduced.

$$\mathbf{A}_i = (\mathbf{A}_i)_{\mathbf{q}_r} \otimes_3 \mathbf{q}^i_r \tag{5}$$

where $(\mathbf{A}_i)_{\mathbf{q}_r} \in \mathbb{R}^{3\times 3\times 12}$ is a constant third order multidimensional matrix, described in section 2.1. The equation will be useful for the gravity forces and mass matrix derivations in sections 3.2 and 3.3.

The velocity of point P can be followed from (4):

$$\dot{\mathbf{r}}^i_P = \dot{\mathbf{r}}^i_{r,P} + \dot{\mathbf{r}}^i_{f,P} = \left(\bar{\mathbf{C}}^i_P + (\mathbf{A}_i)_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}^i_{f,P}\right)\dot{\mathbf{q}}^i_r + \mathbf{A}_i\bar{\boldsymbol{\varphi}}^i_P\dot{\mathbf{q}}^i_f = \mathbf{L}^i_P\dot{\mathbf{q}}^i \tag{6}$$

$$\dot{\mathbf{A}}_i\bar{\mathbf{r}}^i_{f,P} = \left((\mathbf{A}_i)_{\mathbf{q}_r} \otimes_3 \dot{\mathbf{q}}^i_r\right)\bar{\mathbf{r}}^i_{f,P} = \left((\mathbf{A}_i)_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}^i_{f,P}\right)\dot{\mathbf{q}}^i_r \tag{7}$$

where $(\mathbf{A}_i)_{\mathbf{q}_r} \in \mathbb{R}^{3\times 3\times 12}$ is a constant third order matrix, $\otimes_k$ represents a product involving the dimension k of the left operand and

$$\mathbf{L}^i_P = \left(\mathbf{D}^i_P\mathbf{q}^i\right)_{\mathbf{q}^i} = \left[\bar{\mathbf{C}}^i_P + (\mathbf{A}_i)_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}^i_{f,P}\ \ \mathbf{A}_i\bar{\boldsymbol{\varphi}}^i_P\right] \tag{8}$$

Finally, the accelerations, obtained taking derivatives in (6), complete the kinematic description of rigid and flexible bodies.

$$\begin{aligned}\ddot{\mathbf{r}}^i_P = \ddot{\mathbf{r}}^i_{r,P} + \ddot{\mathbf{r}}^i_{f,P} = \left(\bar{\mathbf{C}}^i_P + (\mathbf{A}_i)_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}^i_{f,P}\right) \ddot{\mathbf{q}}^i_r + \mathbf{A}_i \bar{\boldsymbol{\varphi}}^i_P \ddot{\mathbf{q}}^i_f + \\ + \left((\mathbf{A}_i)_{\mathbf{q}_r} \otimes_2 \dot{\bar{\mathbf{r}}}^i_{f,P}\right) \dot{\mathbf{q}}^i_r + \dot{\mathbf{A}}_i \bar{\boldsymbol{\varphi}}^i_P \dot{\mathbf{q}}^i_f = \mathbf{L}^i_P \ddot{\mathbf{q}}^i + \dot{\mathbf{L}}^i_P \dot{\mathbf{q}}^i\end{aligned} \tag{9}$$

$$\dot{\mathbf{L}}^i_P = \left[\left((\mathbf{A}_i)_{\mathbf{q}_r} \otimes_2 \bar{\boldsymbol{\varphi}}^i_P\right) \otimes_2 \dot{\mathbf{q}}^i_f \;\; \left((\mathbf{A}_i)_{\mathbf{q}_r} \otimes_2 \bar{\boldsymbol{\varphi}}^i_P\right) \otimes_3 \dot{\mathbf{q}}^i_r\right] \tag{10}$$

Expanded expressions and more detailed derivations for the kinematics of flexible bodies in natural coordinates are provided in the next section.

2.1 Additional kinematic relations in natural coordinates

Equation (4) is valid for both points and vectors, just defining $\bar{\mathbf{C}}^i_P$ as follows:

$$\begin{aligned}\mathbf{r}^i_{r,P} = \bar{\mathbf{C}}^i_P \mathbf{q}^i_r = \begin{bmatrix}\bar{c}^P_0\mathbf{I}_3 \; \bar{c}^P_1\mathbf{I}_3 \; \bar{c}^P_2\mathbf{I}_3 \; \bar{c}^P_3\mathbf{I}_3\end{bmatrix} \begin{bmatrix}\mathbf{r}^i_0 \\ \mathbf{x}^i_1 \\ \mathbf{x}^i_2 \\ \mathbf{x}^i_3\end{bmatrix} = \begin{bmatrix}\mathbf{r}^i_0 \, \mathbf{x}^i_1 \, \mathbf{x}^i_2 \, \mathbf{x}^i_3\end{bmatrix} \begin{bmatrix}\bar{c}^P_0 \\ \bar{c}^P_1 \\ \bar{c}^P_2 \\ \bar{c}^P_3\end{bmatrix} = \\ = \begin{bmatrix}\mathbf{r}^i_0 \;\; \mathbf{X}^i_3\end{bmatrix} \begin{bmatrix}\bar{c}^P_0 \\ \bar{\mathbf{c}}^3_P\end{bmatrix} = \mathbf{X}^i_4 \bar{\mathbf{c}}_P\end{aligned} \tag{11}$$

$$\bar{c}^P_0 = b^P_0 + b^i_1 \bar{c}^P_1 + b^i_2 \bar{c}^P_2 + b^i_3 \bar{c}^P_3 = b^P_0 + \mathbf{b}^{\mathrm{T}}_i \bar{\mathbf{c}}^3_P \tag{12}$$

$$b^P_0 = \begin{cases} 1 & \text{if } P \text{ is a point} \\ 0 & \text{if } P \text{ is a vector}\end{cases} \tag{13}$$

$$b^i_j = \begin{cases} -1 & \text{if } \mathbf{x}^i_j \text{ is a point} \\ 0 & \text{if } \mathbf{x}^i_j \text{ is a vector}\end{cases} \quad ; \quad j = 1, 2, 3. \tag{14}$$

with $\bar{\mathbf{c}}_P \in \mathbb{R}^4$ the vector of linear combination coefficients associated to the rigid body motion; $\mathbf{X}^i_4 = \begin{bmatrix}\mathbf{r}^i_0 \;\; \mathbf{X}^i_3\end{bmatrix} \in \mathbb{R}^{3\times 4}$ is the point/vector basis of the body in the global frame, composed of the reference point $\mathbf{r}^i_0$ and three points or vectors $\mathbf{X}^i_3 = \begin{bmatrix}\mathbf{x}^i_1 \; \mathbf{x}^i_2 \; \mathbf{x}^i_3\end{bmatrix} \in \mathbb{R}^{3\times 3}$; the scalar b^P_0 and vector $\mathbf{b}_i = \begin{bmatrix}b^i_1 \; b^i_2 \; b^i_3\end{bmatrix}^{\mathrm{T}}$ determine if the magnitudes involved are points or vectors.

The calculation of the linear combination coefficients $\bar{\mathbf{c}}_P = \left[\bar{c}^P_0 \; \left(\bar{\mathbf{c}}^3_P\right)^{\mathrm{T}}\right]^{\mathrm{T}}$ is straightforward from the relations in local coordinates:

$$\begin{aligned}\bar{\mathbf{r}}^i_{r,P} = \bar{\mathbf{C}}^i_P \bar{\mathbf{q}}^i_r = \bar{\mathbf{X}}^i_4 \bar{\mathbf{c}}_P = \bar{c}^P_0 \bar{\mathbf{r}}^i_0 + \bar{\mathbf{X}}^i_3 \bar{\mathbf{c}}^3_P = \left(b^P_0 + \mathbf{b}^{\mathrm{T}}_i \bar{\mathbf{c}}^3_P\right) \bar{\mathbf{r}}^i_0 + \bar{\mathbf{X}}^i_3 \bar{\mathbf{c}}^3_P = \\ = b^P_0 \bar{\mathbf{r}}^i_0 + \left(\bar{\mathbf{X}}^i_3 + \bar{\mathbf{r}}^i_0 \mathbf{b}^{\mathrm{T}}_i\right) \bar{\mathbf{c}}^3_P\end{aligned} \tag{15}$$

Equation (15) can be solved for the coefficients $\bar{\mathbf{c}}^3_P = \begin{bmatrix}\bar{c}^P_1 \; \bar{c}^P_2 \; \bar{c}^P_3\end{bmatrix}^{\mathrm{T}} \in \mathbb{R}^3$ and $\bar{c}^P_0$ obtained by (12):

$$\bar{\mathbf{c}}^3_P = \bar{\mathbf{X}}^{-1}_i \left(\bar{\mathbf{r}}^i_P - b^P_0 \bar{\mathbf{r}}^i_0\right) \tag{16}$$

$$\bar{\mathbf{X}}_i = \bar{\mathbf{X}}_3^i + \bar{\mathbf{r}}_0^i \mathbf{b}^{\mathrm{T}} = \begin{bmatrix} \bar{\mathbf{v}}_1^i & \bar{\mathbf{v}}_2^i & \bar{\mathbf{v}}_3^i \end{bmatrix} \tag{17}$$

where $\bar{\mathbf{X}}_i \in \mathbb{R}^{3\times 3}$ is the vector basis of the body in the local reference frame which is always composed of 3 vectors: if $\bar{\mathbf{x}}_j^i$ is a vector then $\bar{\mathbf{v}}_j^i = \bar{\mathbf{x}}_j^i + b_j^i \bar{\mathbf{r}}_0^i = \bar{\mathbf{x}}_j^i$ (If the three entities $\bar{\mathbf{x}}_1^i$, $\bar{\mathbf{x}}_2^i$, $\bar{\mathbf{x}}_3^i$ are vectors, the bases $\bar{\mathbf{X}}_3^i$ and $\bar{\mathbf{X}}_i$ are identical); if $\bar{\mathbf{x}}_j^i$ is a point then a vector is formed with the reference point $\bar{\mathbf{v}}_j^i = \bar{\mathbf{x}}_j^i + b_j^i \bar{\mathbf{r}}_0^i = \bar{\mathbf{x}}_j^i - \bar{\mathbf{r}}_0^i$. Matrix $\bar{\mathbf{X}}_i^{-1}$ is guaranteed to exist if a set of natural coordinates $\mathbf{q}_r^i$, properly representing the three directions of the local space is chosen. This kinematic description is more general than those presented in previous works for natural coordinates and very convenient if a general implementation is aimed.

The rotation matrix of the body can be built by expressing the vector basis (17) in the global reference frame:

$$\mathbf{X}_i = \mathbf{A}_i \bar{\mathbf{X}}_i \Rightarrow \mathbf{A}_i = \mathbf{X}_i \bar{\mathbf{X}}_i^{-1} \tag{18}$$

Then, the time derivative of the rotation matrix can also be expressed as any of the following:

$$\dot{\mathbf{A}}_i = (\mathbf{A}_i)_{\mathbf{q}_r} \otimes_3 \dot{\mathbf{q}}_r^i = \left((\mathbf{X}_i)_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{X}}_i^{-1} \right) \otimes_3 \dot{\mathbf{q}}_r^i = \dot{\mathbf{X}}_i \bar{\mathbf{X}}_i^{-1} \tag{19}$$

$$\dot{\mathbf{X}}_i = (\mathbf{X}_i)_{\mathbf{q}_r} \otimes_3 \dot{\mathbf{q}}_r^i = \dot{\mathbf{X}}_3^i + \dot{\mathbf{r}}_0^i \mathbf{b}_i^{\mathrm{T}} \tag{20}$$

$$(\mathbf{A}_i)_{\mathbf{q}_r} = (\mathbf{X}_i)_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{X}}_i^{-1} \tag{21}$$

where $(\mathbf{X}_i)_{\mathbf{q}_r} \in \mathbb{R}^{3\times 3\times 12}$ is a constant third order multidimensional matrix with the following expression,

$$(\mathbf{X}_i)_{\mathbf{q}_r} = \left[\mathbf{E} \otimes_2 \mathbf{b}_i^{\mathrm{T}} \;|_3\; \mathbf{E} \otimes_2 \mathbf{e}_1^{\mathrm{T}} \;|_3\; \mathbf{E} \otimes_2 \mathbf{e}_2^{\mathrm{T}} \;|_3\; \mathbf{E} \otimes_2 \mathbf{e}_3^{\mathrm{T}} \right] \tag{22}$$

$$\mathbf{e}_1^{\mathrm{T}} = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix};\; \mathbf{e}_2^{\mathrm{T}} = \begin{bmatrix} 0 & 1 & 0 \end{bmatrix};\; \mathbf{e}_3^{\mathrm{T}} = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix} \tag{23}$$

and $\mathbf{E} = \left[\mathbf{e}_1 \,|_3\, \mathbf{e}_2 \,|_3\, \mathbf{e}_3 \right] \in \mathbb{R}^{3\times 1\times 3}$ is a third order multidimensional matrix, considering $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \in \mathbb{R}^{3\times 1}$ matrices, with the second dimension equal to 1. Each column in the first equality (22) is a $3\times 3\times 3$ matrix and each column in the second identity is a 3×3 matrix; the concatenation is always in the third dimension, giving rise to the $3\times 3\times 12$ matrix; the compact form in the last equality uses the T1 transpose operator (switching dimensions 2 and 3).

Finally, observe that, as pointed out in (5), the relation between the rotation matrix and the rigid body natural coordinates is also linear, because:

$$\mathbf{X}_i = (\mathbf{X}_i)_{\mathbf{q}_r} \otimes_3 \mathbf{q}_r^i \Rightarrow \mathbf{A}_i = \left((\mathbf{X}_i)_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{X}}_i^{-1} \right) \otimes_3 \mathbf{q}_r^i = (\mathbf{A}_i)_{\mathbf{q}_r} \otimes_3 \mathbf{q}_r^i \tag{24}$$

The kinematic description provided in this work is general for points or vectors. If $\mathbf{r}_P^i$ is a flexible vector instead o a flexible point, the equations also hold but its flexible deformation requires from the mode shape matrix of the vector as well.

3 Equations of motion: ALI3-P FFR formulation in natural coordinates

Elaborating on Lagrange's equations, the index-3 DAE equations of motion in natural coordinates can be derived, which, in turn, can be converted to an equivalent index-3 DAE augmented Lagrangian system of equations, [12], enforcing the dynamic equilibrium of forces at time step $n+1$ and the constraints satisfaction at position level:

$$\left[\mathbf{M}\ddot{\mathbf{q}}^{*}+\mathbf{K}^{e}\mathbf{q}+\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\left(\boldsymbol{\lambda}^{*}+\boldsymbol{\alpha}\boldsymbol{\Phi}\right)\right]_{n+1}^{\{i\}}=\mathbf{Q}_{n+1}^{\{i\}}+\mathbf{Q}_{n+1}^{v\{i\}} \tag{25a}$$

$$\mathbf{Q}^{v}=-\dot{\mathbf{M}}\dot{\mathbf{q}}^{*}+\frac{1}{2}\left(\mathbf{M}_{\mathbf{q}}\otimes_{2}\dot{\mathbf{q}}^{*}\right)^{\mathrm{T}}\dot{\mathbf{q}}^{*} \tag{25b}$$

$$\boldsymbol{\lambda}_{n+1}^{*\{i+1\}}=\boldsymbol{\lambda}_{n+1}^{*\{i\}}+\boldsymbol{\alpha}\boldsymbol{\Phi}_{n+1}^{\{i\}},\ i=1,2,... \tag{25c}$$

Where $\mathbf{Q}^{v}-\mathbf{M}\ddot{\mathbf{q}}^{*}$ represents the inertia forces, $-\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\left(\boldsymbol{\lambda}^{*}+\boldsymbol{\alpha}\boldsymbol{\Phi}\right)$ the constraints generalized internal forces with $\boldsymbol{\alpha}$ a diagonal matrix of penalty factors for each constraint equation, $-\mathbf{K}^{e}\mathbf{q}$ are the internal elastic forces and the remaining forces are included in the external generalized forces vector, $\mathbf{Q}$. Moreover, $\{i\}$ is the iteration index of the approximate Lagrange multipliers, $\boldsymbol{\lambda}^{*}$, which are converged together by (25c) with the equilibrium equations (25a) at each time step.

For rigid body multibody systems modeled in natural coordinates it is easy to arrive at a constant mass matrix (and this is a common assumption), thus the velocity dependent generalized forces $\mathbf{Q}_{v}$ vanish, as well as the term $\mathbf{K}^{e}\mathbf{q}$ coming from the elastic potential, which is not present. A constant mass matrix is also possible for flexible bodies but at the expense of some assumptions and a good number of extra variables and constraints [25] and therefore it will not be the approach adopted in this work.

Projections of velocities and accelerations onto the constraints manifolds are among the most effective techniques for stabilizing the constraints in index-3 DAE schemes. The magnitudes $\dot{\mathbf{q}}^{*}$ and $\ddot{\mathbf{q}}^{*}$ stand for unprojected velocities and accelerations coming from the solution of equations (25), which have to be projected onto the constraints manifolds, to obtain the final, projected, velocities and accelerations $\dot{\mathbf{q}}$ and $\ddot{\mathbf{q}}$:

$$\left(\bar{\mathbf{P}}+\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\varsigma\boldsymbol{\alpha}\boldsymbol{\Phi}_{\mathbf{q}}\right)_{n+1}\dot{\mathbf{q}}_{n+1}=\left[\bar{\mathbf{P}}\dot{\mathbf{q}}^{*}-\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\varsigma\alpha\boldsymbol{\Phi}_{t}\right]_{n+1} \tag{26}$$

$$\left(\bar{\mathbf{P}}+\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\varsigma\boldsymbol{\alpha}\boldsymbol{\Phi}_{\mathbf{q}}\right)_{n+1}\ddot{\mathbf{q}}_{n+1}=\left[\bar{\mathbf{P}}\ddot{\mathbf{q}}^{*}-\boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}}\left(\varsigma\boldsymbol{\alpha}\left(\dot{\boldsymbol{\Phi}}_{\mathbf{q}}\dot{\mathbf{q}}+\dot{\boldsymbol{\Phi}}_{t}\right)\right)\right]_{n+1} \tag{27}$$

with $\varsigma\boldsymbol{\alpha}$ the penalty parameters for the projections of velocities and accelerations and $\bar{\mathbf{P}}$ is a symmetric projection matrix. The projection equations (26) and (27) are the non-iterative penalty projections of velocities and accelerations thoroughly derived and explained in [14]. A common choice is $\bar{\mathbf{P}}=\mathbf{M}$ and values of ς in the range of 10^{-5} to 1 can give good results, depending on the numerical conditioning, satisfaction of constraints and levels of energy numerical dissipation required [26, **?**].

3.1 Flexible body constraints

The addition of flexible points and vectors to the generalized coordinates of the system, $\mathbf{q}$, is very convenient, among other reasons, to make it possible sharing points/vectors between bodies (typical way of defining kinematic joints in natural coordinates) or to make use of kinematic constraints involving points and vectors (which can be either rigid or flexible).

The addition of the coordinates of a flexible point or vector as generalized coordinates, requires adding three kinematic constraints relating the new coordinates to the rigid, $\mathbf{q}_r^i$, and flexible, $\mathbf{q}_f^i$, body coordinates of the body.

The constraints for points represent the kinematic equation (4):

$$\boldsymbol{\Phi}_P = \mathbf{r}_P^i - \mathbf{r}_{r,P}^i - \mathbf{r}_{f,P}^i = \mathbf{r}_P^i - \bar{\mathbf{C}}_P^i \mathbf{q}_r^i - \mathbf{A}_i \bar{\boldsymbol{\varphi}}_P^i \mathbf{q}_f^i = \mathbf{r}_P^i - \mathbf{D}_P^i \mathbf{q}^i \tag{28}$$

The contribution of the constraint to the Jacobian matrix $\boldsymbol{\Phi}_\mathbf{q}$ is given by the following blocks:

$$(\boldsymbol{\Phi}_P)_\mathbf{q} = \begin{bmatrix} \dfrac{\partial \boldsymbol{\Phi}_P}{\partial \mathbf{r}_P^i} & \dfrac{\partial \boldsymbol{\Phi}_P}{\partial \mathbf{q}^i} \end{bmatrix} = \begin{bmatrix} \mathbf{I}_3 & -\mathbf{L}_P^i \end{bmatrix} \tag{29}$$

where equation (8) has been used.

For the dynamics, the time derivative of the Jacobian matrix times velocities is also required,

$$\left(\dot{\boldsymbol{\Phi}}_P\right)_\mathbf{q} \dot{\mathbf{q}} = -\dot{\mathbf{L}}_P^i \dot{\mathbf{q}}^i = -\left((\mathbf{A}_i)_{\mathbf{q}_r} \otimes_2 \ddot{\bar{\mathbf{r}}}_{f,P}^i\right) \dot{\mathbf{q}}_r^i - \dot{\mathbf{A}}_i \bar{\boldsymbol{\varphi}}_P^i \dot{\mathbf{q}}_f^i = -2\dot{\mathbf{A}}_i \bar{\boldsymbol{\varphi}}_P^i \dot{\mathbf{q}}_f^i \tag{30}$$

3.2 External forces and gravity potential

The application of an external force $\mathbf{F}$ on point P (of body i) is given by:

$$\mathbf{Q}_{F,P}^i = \left(\frac{\partial \mathbf{r}_P^i}{\partial \mathbf{q}^i}\right)^{\mathrm{T}} \mathbf{F} = \mathbf{L}_P^{i\mathrm{T}} \mathbf{F} \tag{31}$$

Gravitational are a special type of volumetric forces which can either be obtained from the gravity potential[1] or from direct application of equation (31) to the differential gravitational forces $\mathrm{d}\mathbf{F}_v = \mathbf{g}\mathrm{d}m$:

$$\mathbf{Q}_g^i = \int_i \mathbf{L}^{\mathrm{T}} \mathrm{d}\mathbf{F}_v = \int_i \begin{bmatrix} \left(\bar{\mathbf{C}} + \mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f\right)^{\mathrm{T}} \\ \left(\mathbf{A}\bar{\boldsymbol{\varphi}}\right)^{\mathrm{T}} \end{bmatrix} \mathbf{g}\mathrm{d}m \tag{32}$$

Elaborating on (32), the gravitational generalized forces can be expressed as the sum of the constant rigid-body term and an additional term linear with the coordinates.

$$\mathbf{Q}_g^i = \begin{bmatrix} \mathbf{Q}_{r,g}^i \\ \mathbf{0}_{n_f^i} \end{bmatrix} - \mathbf{K}_g^i \mathbf{q}^i \tag{33}$$

[1] From the gravity potential, the same expression is obtained $V_g^i = \int_i \mathbf{r}^{\mathrm{T}} \mathbf{g}\mathrm{d}m \Rightarrow \mathbf{Q}_g^i = \dfrac{\mathrm{d}V_g^i}{\mathrm{d}\mathbf{q}} = \int_i \mathbf{L}^{\mathrm{T}} \mathbf{g}\mathrm{d}m$

$$\mathbf{Q}^i_{r,g} = \left(\int_i \bar{\mathbf{C}}^{\mathrm{T}} \mathrm{d}m \right) \mathbf{g} = m_i \bar{\mathbf{C}}^{i\mathrm{T}}_G \mathbf{g} \tag{34}$$

$$\mathbf{K}^i_g = - \begin{bmatrix} \mathbf{0}_{12\times 12} & \left[\mathbf{g}^{\mathrm{T}} \left((\mathbf{X}_i)_{\mathbf{q}_r} \otimes_2 \mathbf{i}^{\bar{\mathbf{X}}_i}_1 \right) \right]^{\mathrm{T}} \\ \mathbf{g}^{\mathrm{T}} \left((\mathbf{X}_i)_{\mathbf{q}_r} \otimes_2 \mathbf{i}^{\bar{\mathbf{X}}_i}_1 \right) & \mathbf{0}_{n^i_f \times n^i_f} \end{bmatrix} \tag{35}$$

$$\mathbf{i}^{\bar{\mathbf{X}}_i}_1 = \bar{\mathbf{X}}^{-1}_i \mathbf{i}^i_1 \tag{36}$$

$$\mathbf{i}^i_1 = \int_i \bar{\boldsymbol{\varphi}} \mathrm{d}m \tag{37}$$

Term $\mathbf{Q}^i_{r,g}$ is the rigid-body generalized gravity forces vector, the only contribution if body i is rigid. Integral $\mathbf{i}^i_1 \in \mathbb{R}^{3\times n^i_f}$ is constant during the whole simulation, so do matrices $\mathbf{i}^{\bar{\mathbf{X}}_i}_1 \in \mathbb{R}^{3\times n^i_f}$ and $\mathbf{K}^i_g \in \mathbb{R}^{n^i \times n^i}$, which can be precalculated and stored.

3.3 Kinetic energy of a flexible body in natural coordinates: mass matrix

A continuum mechanics approach is used in this work for building the mass matrix, resulting in the derivation of only six invariant shape integrals, on top of which the mass matrix of each flexible body can be efficiently built in each time step. This is a reduced number of shape integrals, compared to previous works, because of the simplifications adopted and particularization for the kinematics in natural coordinates and the profuse use of multidimensional algebra.

Using equation (6), the kinetic energy of flexible body i, reads:

$$T_i = \frac{1}{2} \int_i \dot{\mathbf{r}}^{\mathrm{T}} \dot{\mathbf{r}} \mathrm{d}m = \frac{1}{2} \dot{\mathbf{q}}^{i\mathrm{T}} \left(\int_i \mathbf{L}^{\mathrm{T}} \mathbf{L} \mathrm{d}m \right) \dot{\mathbf{q}}^i = \frac{1}{2} \dot{\mathbf{q}}^{i\mathrm{T}} \mathbf{M}_i \dot{\mathbf{q}}^i \tag{38}$$

$$\mathbf{M}_i = \int_i \begin{bmatrix} \left(\bar{\mathbf{C}} + \mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f \right)^{\mathrm{T}} \\ \bar{\boldsymbol{\varphi}}^{\mathrm{T}} \mathbf{A}^{\mathrm{T}} \end{bmatrix} \left[\bar{\mathbf{C}} + \mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f \;\; \mathbf{A} \bar{\boldsymbol{\varphi}} \right] \mathrm{d}m = \begin{bmatrix} \mathbf{M}_{rr} & \mathbf{M}_{rf} \\ \mathbf{M}_{fr} & \mathbf{M}_{ff} \end{bmatrix} \tag{39}$$

The global mass matrix $\mathbf{M}$ is a sparse block-diagonal matrix, formed with the elemental mass matrices, $\mathbf{M}_i$, of the bodies. The integrals in (39) are profusely derived in appendix B, only final results are provided here.

The expressions of the mass matrix blocks presented next, have been derived with some important constraints but pose important advantages: first, the expressions are general, for their implementation in MBSLIM; second, all the terms are built to be constant, linear or bi-linear with the states, thus most of the magnitudes are precalculated and stored, such as only products with the states are needed for computing the mass matrix in each time instant and makes the sensitivities very easy to obtain; third, tensor or multidimensional matrix algebra is profusely employed with the aim of minimizing the number of terms needed and reusing them from the dynamics in the sensitivity analysis and from one particular formulation into others.

In other works, like

3.3.1 Mass matrix: rigid-rigid block ($\mathbf{M}_{rr}$)

Block, $\mathbf{M}_{rr}$, can be expanded in four terms:

$$\begin{aligned}\mathbf{M}_{rr} &= \int_i \left(\bar{\mathbf{C}} + \mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f\right)^{\mathrm{T}} \left(\bar{\mathbf{C}} + \mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f\right) \mathrm{d}m \\ &= \mathbf{M}_{rr1} + \mathbf{M}_{rr2} + \mathbf{M}_{rr2}^{\mathrm{T}} + \mathbf{M}_{rr4}\end{aligned} \tag{40}$$

All the integrals in (40), are derived in appendix B.1. The first term $\mathbf{M}_{rr1}$ is constant for each simulation, the second an third terms $\mathbf{M}_{rr2}$, $\mathbf{M}_{rr2}^{\mathrm{T}}$ are linear with the flexible coordinates of the body and the fourth one, $\mathbf{M}_{rr4}$ is bi-linear with the flexible coordinates, $\mathbf{q}_f^i$.

The first term, $\mathbf{M}_{rr1} = \int_i \bar{\mathbf{C}}^{\mathrm{T}} \bar{\mathbf{C}} \mathrm{d}m$ is the constant 12×12 rigid body mass matrix in natural coordinates:

$$\mathbf{M}_{rr1} = \int_i \bar{\mathbf{C}}^{\mathrm{T}} \bar{\mathbf{C}} \mathrm{d}m = \int_i \begin{bmatrix} \bar{c}_0^2 \mathbf{I}_3 & \bar{c}_0 \bar{c}_k \mathbf{I}_3 \\ \bar{c}_j \bar{c}_0 \mathbf{I}_3 & \bar{c}_j \bar{c}_k \mathbf{I}_3 \end{bmatrix} \mathrm{d}m;\ j,k = 1,2,3. \tag{41}$$

where each 3×3 diagonal block is formed with one element of the following 4×4 matrix[2]:

$$\begin{aligned}\mathbf{M}_{rr1}^{4\times4} &= \int_i \bar{\mathbf{c}}\bar{\mathbf{c}}^{\mathrm{T}} \mathrm{d}m = \int_i \bar{\mathbf{c}} \otimes \bar{\mathbf{c}} \mathrm{d}m = \int_i \begin{bmatrix} \bar{c}_0^2 & \bar{c}_0 \bar{\mathbf{c}}^{3\mathrm{T}} \\ \bar{\mathbf{c}}^3 \bar{c}_0 & \bar{\mathbf{c}}^3 \bar{\mathbf{c}}^{3\mathrm{T}} \end{bmatrix} \mathrm{d}m = \\ &= \begin{bmatrix} m_i + \mathbf{b}_i^{\mathrm{T}} \bar{\mathbf{X}}_i^{-1} \left[\bar{\mathbf{P}}_0^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \mathbf{b}_i + 2m_i \left(\bar{\mathbf{r}}_{r,G}^i - \bar{\mathbf{r}}_0^i\right)\right] & SYMM \\ \bar{\mathbf{X}}_i^{-1} \left[m_i \left(\bar{\mathbf{r}}_{r,G}^i - \bar{\mathbf{r}}_0^i\right) + \bar{\mathbf{P}}_0^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \mathbf{b}_i\right] & \bar{\mathbf{X}}_i^{-1} \bar{\mathbf{P}}_0^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \end{bmatrix}\end{aligned} \tag{42}$$

with G the body center of mass and thus $\bar{\mathbf{r}}_{r,G}^i$ the rigid-body center of mass local coordinates, $\bar{\mathbf{P}}_0^i$ the planar inertia tensor [3]:

$$\bar{\mathbf{P}}_0^i = \int_i \left(\bar{\mathbf{r}}_r - \bar{\mathbf{r}}_0\right) \left(\bar{\mathbf{r}}_r - \bar{\mathbf{r}}_0\right)^{\mathrm{T}} \mathrm{d}m \tag{43}$$

The second and third terms, $\mathbf{M}_{rr2}$ and $\mathbf{M}_{rr3} = \mathbf{M}_{rr2}^{\mathrm{T}}$ give a symmetric contribution, linearly dependent with the flexible coordinates:

$$\begin{aligned}\mathbf{M}_{rr2} + \mathbf{M}_{rr2}{}^{\mathrm{T}} &= \int_i \bar{\mathbf{C}}^{\mathrm{T}} \mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f \mathrm{d}m + \left[\int_i \bar{\mathbf{C}}^{\mathrm{T}} \mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f \mathrm{d}m\right]^{\mathrm{T}} = \\ &= \begin{bmatrix} 2m_{rr2}^{00} \mathbf{I}_3 & \left(m_{rr2}^{0k} + m_{rr2}^{k0}\right) \mathbf{I}_3 \\ \left(m_{rr2}^{j0} + m_{rr2}^{0j}\right) \mathbf{I}_3 & \left(m_{rr2}^{jk} + m_{rr2}^{kj}\right) \mathbf{I}_3 \end{bmatrix};\ j,k = 1,2,3.\end{aligned} \tag{44}$$

[2] The 4×4 format has advantages in terms of implementation with respect to the 12×12 format because products involving the block are cheaper and memory storage is reduced.

[3] $\bar{\mathbf{P}}_0^i$ is related to the inertia tensor w.r.t. $\bar{\mathbf{r}}_0^i$ by: $\bar{\mathbf{P}}_0^i = J_0^i \mathbf{I}_3 - \bar{\mathbf{J}}_0^i = \frac{\mathrm{tr}\left(\bar{\mathbf{J}}_0^i\right)}{2} \mathbf{I}_3 - \bar{\mathbf{J}}_0^i$, with J_0^i the mass moment of inertia w.r.t. $\bar{\mathbf{r}}_0^i$ and tr the trace of a matrix. $\bar{\mathbf{J}}_0^i$ can be expressed in terms of the inertia tensor in the center of mass (the most common one) by means of Steiner's theorem.

where each 3×3 diagonal block in equation (44) is formed with one element of the following 4×4 matrix:

$$\mathbf{M}_{rr2}^{4\times4} = \begin{bmatrix} m_{rr2}^{00} & m_{rr2}^{01} & m_{rr2}^{02} & m_{rr2}^{03} \\ m_{rr2}^{10} & m_{rr2}^{11} & m_{rr2}^{12} & m_{rr2}^{13} \\ m_{rr2}^{20} & m_{rr2}^{21} & m_{rr2}^{22} & m_{rr2}^{23} \\ m_{rr2}^{30} & m_{rr2}^{31} & m_{rr2}^{32} & m_{rr2}^{33} \end{bmatrix} = \begin{bmatrix} m_{rr2}^{00} & \left(\mathbf{m}_{rr2}^{\mathbf{30}}\right)^{\mathrm{T}} \\ \left(\mathbf{m}_{rr2}^{\mathbf{03}}\right)^{\mathrm{T}} & \left(\mathbf{M}_{rr2}^{33}\right)^{\mathrm{T}} \end{bmatrix} \tag{45a}$$

$$m_{rr2}^{00} = \mathbf{b}_i^{\mathrm{T}} \left(\mathbf{i}_1^{\bar{\mathbf{X}}_i} + \mathbf{i}_2^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{b}_i\right) \mathbf{q}_f^i = \left(m_{rr2}^{00}\right)_{\mathbf{q}_f^i} \mathbf{q}_f^i \tag{45b}$$

$$\mathbf{m}_{rr2}^{\mathbf{03}} = \left(\mathbf{b}_i^{\mathrm{T}} \mathbf{i}_2^{\bar{\mathbf{X}}_i}\right) \mathbf{q}_f^i = \left(\mathbf{m}_{rr2}^{\mathbf{03}}\right)_{\mathbf{q}_f^i} \mathbf{q}_f^i \tag{45c}$$

$$\mathbf{m}_{rr2}^{\mathbf{30}} = \left(\mathbf{i}_1^{\bar{\mathbf{X}}_i} + \mathbf{i}_2^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{b}_i\right) \mathbf{q}_f^i = \left(\mathbf{m}_{rr2}^{\mathbf{30}}\right)_{\mathbf{q}_f^i} \mathbf{q}_f^i \tag{45d}$$

$$\mathbf{M}_{rr2}^{33} = \mathbf{i}_2^{\bar{\mathbf{X}}_i} \otimes_3 \mathbf{q}_f^i = \left(\mathbf{M}_{rr2}^{33}\right)_{\mathbf{q}_f^i} \otimes_3 \mathbf{q}_f^i \tag{45e}$$

$$\mathbf{i}_2^{\bar{\mathbf{X}}_i} = \bar{\mathbf{X}}_i^{-1} \mathbf{i}_2^i \otimes_2 \bar{\mathbf{X}}_i^{-\mathrm{T}} \tag{45f}$$

$$\mathbf{i}_2^i = \int_i \left(\bar{\boldsymbol{\varphi}} \otimes (\bar{\mathbf{r}} - \bar{\mathbf{r}}_0)\right)^{\mathrm{T}_1} \mathrm{d}m \tag{45g}$$

where $\mathbf{i}_2^i \in \mathbb{R}^{3\times3\times n_f^i}$ and $\mathbf{i}_2^{\bar{\mathbf{X}}_i} \in \mathbb{R}^{3\times3\times n_f^i}$ are constant multidimensional matrices for each simulation and everything else in equations (45) is constant as well, except for the flexible states, $\mathbf{q}_f^i$. Equations (45c) and (45d) give vectors in $\mathbb{R}^3$ as a result, nevertheless terms $\mathbf{m}_{rr2}^{\mathbf{03}} \in \mathbb{R}^{1\times3}$ and $\mathbf{m}_{rr2}^{\mathbf{30}} \in \mathbb{R}^{3\times1}$ are considered matrices in order to be assembled in (45a).

Moreover, the integral $\mathbf{i}_2^i$ can be further decomposed as:

$$\mathbf{i}_2^i = \mathbf{i}_4^i - \left(\mathbf{i}_1^i \otimes \bar{\mathbf{r}}_0\right)^{\mathrm{T}_1} \tag{46}$$

$$\mathbf{i}_4^i = \int_i \left(\bar{\boldsymbol{\varphi}} \otimes \bar{\mathbf{r}}\right)^{\mathrm{T}_1} \mathrm{d}m \tag{47}$$

Observe that all the blocks in equation (45) are linear in $\mathbf{q}_f^i$, therefore:

$$\mathbf{M}_{rr2} + \mathbf{M}_{rr2}{}^{\mathrm{T}} = \left(\mathbf{M}_{rr2} + \mathbf{M}_{rr2}{}^{\mathrm{T}}\right)_{\mathbf{q}_f^i} \otimes_3 \mathbf{q}_f^i \tag{48}$$

wherein $\left(\mathbf{M}_{rr2} + \mathbf{M}_{rr2}{}^{\mathrm{T}}\right)_{\mathbf{q}_f^i} \in \mathbb{R}^{12\times12\times n_f^i}$ is the constant multidimensional matrix expressed in (61).

The fourth term $\mathbf{M}_{rr4}$ has a bilinear dependence with $\mathbf{q}_f$:

$$\mathbf{M}_{rr4} = \int_i \left(\mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f\right)^{\mathrm{T}} \left(\mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f\right) \mathrm{d}m = \begin{bmatrix} m_{rr4}^{00}\mathbf{I}_3 & m_{rr4}^{0k}\mathbf{I}_3 \\ m_{rr4}^{j0}\mathbf{I}_3 & m_{rr4}^{jk}\mathbf{I}_3 \end{bmatrix};\ j,k = 1,2,3. \tag{49}$$

Each 3×3 diagonal block in (49) is formed with one element of the following 4×4 matrix:

$$\mathbf{M}_{rr4}^{4\times4} = \begin{bmatrix} m_{rr4}^{00} & m_{rr4}^{01} & m_{rr4}^{02} & m_{rr4}^{03} \\ m_{rr4}^{10} & m_{rr4}^{11} & m_{rr4}^{12} & m_{rr4}^{13} \\ m_{rr4}^{20} & m_{rr4}^{21} & m_{rr4}^{22} & m_{rr4}^{23} \\ m_{rr4}^{30} & m_{rr4}^{31} & m_{rr4}^{32} & m_{rr4}^{33} \end{bmatrix} = \left[\mathbf{T}_{rr4} \otimes_3 \mathbf{q}_f^i\right] \otimes_3 \mathbf{q}_f^i \tag{50a}$$

$$\mathbf{T}_{rr4} = \begin{bmatrix} \mathbf{T}_{rr4}^{\mathbf{00}} \Big|_2 & \mathbf{T}_{rr4}^{\mathbf{30}} \\ \mathbf{T}_{rr4}^{\mathbf{03}} \Big|_2 & \mathbf{i}_3^{\bar{\mathbf{X}}_i} \end{bmatrix} \tag{50b}$$

$$\mathbf{T}_{rr4}^{\mathbf{00}} = \mathbf{b}_i^{\mathrm{T}} \left(\mathbf{i}_3^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{b}_i\right) \tag{50c}$$

$$\mathbf{T}_{rr4}^{\mathbf{03}} = \mathbf{i}_3^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{b}_i \tag{50d}$$

$$\mathbf{T}_{rr4}^{\mathbf{30}} = \mathbf{b}_i^{\mathrm{T}} \mathbf{i}_3^{\bar{\mathbf{X}}_i} \tag{50e}$$

$$\mathbf{i}_3^{\bar{\mathbf{X}}_i} = \bar{\mathbf{X}}_i^{-1} \left(\mathbf{i}_3^i\right)^{\mathrm{T}_{2,4}} \otimes_2 \bar{\mathbf{X}}_i^{-\mathrm{T}} \tag{50f}$$

$$\mathbf{i}_3^i = \int_i \bar{\boldsymbol{\varphi}}^{\mathrm{T}} \otimes \bar{\boldsymbol{\varphi}} \mathrm{d}m \tag{50g}$$

where integrals $\mathbf{i}_3^i \in \mathbb{R}^{n_f^i \times 3 \times 3 \times n_f^i}$, $\mathbf{i}_3^{\bar{\mathbf{X}}_i} \in \mathbb{R}^{3 \times 3 \times n_f^i \times n_f^i}$ are fourth order multidimensional matrices, constant for every simulation, thus, $\mathbf{T}_{rr4} \in \mathbb{R}^{4 \times 4 \times n_f^i \times n_f^i}$ is also a constant four order multidimensional matrix, which appears also in the construction of $\mathbf{M}_{rf}$ in section 3.3.2. The result of equations (50d) and (50e), with reduced tensor products, are third order identical matrices[4] in $\mathbb{R}^{3 \times n_f^i \times n_f^i}$, nevertheless terms $\mathbf{T}_{rr4}^{\mathbf{03}} \in \mathbb{R}^{3 \times 1 \times n_f^i \times n_f^i}$ and $\mathbf{T}_{rr4}^{\mathbf{30}} \in \mathbb{R}^{1 \times 3 \times n_f^i \times n_f^i}$ are considered fourth order matrices to be assembled in (50b) and further operated with. $\mathbf{T}_{rr4}^{\mathbf{00}} \in \mathbb{R}^{1 \times 1 \times n_f^i \times n_f^i}$ is considered a fourth order matrix as well, in the context of equation (50b).

3.3.2 Mass matrix: rigid-flexible ($\mathbf{M}_{fr}$) and flexible-rigid ($\mathbf{M}_{rf}$) blocks

The second and third blocks, $\mathbf{M}_{rf} = \mathbf{M}_{fr}^{\mathrm{T}}$ are thoroughly derived in appendix B.2 and summarized here.

$$\mathbf{M}_{rf} = \int_i \bar{\mathbf{C}}^{\mathrm{T}} \left(\mathbf{A}_{\mathbf{q}_r} \otimes_3 \mathbf{q}_r\right) \bar{\boldsymbol{\varphi}} \mathrm{d}m + \int_i \left(\mathbf{A}_{\mathbf{q}_r} \otimes_2 \left(\bar{\boldsymbol{\varphi}} \mathbf{q}_f\right)\right)^{\mathrm{T}} \mathbf{A} \bar{\boldsymbol{\varphi}} \mathrm{d}m = \mathbf{M}_{rf1} + \mathbf{M}_{rf2} \tag{51}$$

The first term, $\mathbf{M}_{rf1}$, is linear with the rigid body coordinates, $\mathbf{q}_r^i$, and the same constant multidimensional matrix of linear coefficients used in (48):

$$\mathbf{M}_{rf1} = \left(\mathbf{M}_{rr2}\right)_{\mathbf{q}_f^i} \otimes_2 \mathbf{q}_r^i = \left(\mathbf{M}_{rr2}\right)_{\mathbf{q}_f^i}^{\mathrm{T}_1} \otimes_3 \mathbf{q}_r^i \tag{52a}$$

[4] Reduced products result in $\mathbf{T}_{rr4}^{\mathbf{03}} = \mathbf{T}_{rr4}^{\mathbf{30}}$ because of the symmetry properties of $\mathbf{i}_3^i$ and $\mathbf{i}_3^{\bar{\mathbf{X}}_i}$, proved in appendices B.1 and B.2

$$(\mathbf{M}_{rr2})_{\mathbf{q}_f^i} = \begin{bmatrix} \mathbf{I}_3 \otimes \left(m_{rr2}^{00}\right)_{\mathbf{q}_f} & \vert_2 & \mathbf{I}_3 \otimes \left(m_{rr2}^{0k}\right)_{\mathbf{q}_f} \\ \mathbf{I}_3 \otimes \left(m_{rr2}^{j0}\right)_{\mathbf{q}_f} & \vert_2 & \mathbf{I}_3 \otimes \left(m_{rr2}^{jk}\right)_{\mathbf{q}_f} \end{bmatrix} \; j,k = 1,2,3. \tag{52b}$$

Because of equation (5), the second term, $\mathbf{M}_{rf2}$, is bi-linear with the rigid and flexible body coordinates, $\mathbf{q}_r^i$ and $\mathbf{q}_f^i$ and the same constant coefficients appearing in (49) are also present here:

$$\mathbf{M}_{rf2} = \left[(\mathbf{M}_{rf2})_{\mathbf{q}_r^i \mathbf{q}_f^i} \otimes_4 \mathbf{q}_f^i \right] \otimes_3 \mathbf{q}_r^i \tag{53a}$$

$$(\mathbf{M}_{rf2})_{\mathbf{q}_r^i \mathbf{q}_f^i} = \begin{bmatrix} \mathbf{I}_3 \otimes \mathbf{T}_{rr4}^{00} & \vert_2 & \mathbf{I}_3 \otimes \mathbf{T}_{rr4}^{0k} \\ \mathbf{I}_3 \otimes \mathbf{T}_{rr4}^{j0} & \vert_2 & \mathbf{I}_3 \otimes \mathbf{T}_{rr4}^{jk} \end{bmatrix}^{\mathrm{T}_{1,4}} ; \; j,k = 1,2,3. \tag{53b}$$

Each block of size $3 \times n_f \times 3 \times n_f$ in $(\mathbf{M}_{rf2})_{\mathbf{q}_r^i \mathbf{q}_f^i} \in \mathbb{R}^{12 \times n_f^i \times 12 \times n_f^i}$ is built with the outer product of the identity matrix $\mathbf{I}_3 \in \mathbb{R}^{3\times 3}$ times an element of size $1 \times 1 \times n_f^i \times n_f^i$ taken from $\mathbf{T}_{rr4}$ (equation (50b)) and the dimensions 2 and 3 of the result transposed.

3.3.3 Mass matrix: flexible-flexible block ($\mathbf{M}_{ff}^i$)

The fourth (and last) block, $\mathbf{M}_{ff}^i$ is constant:

$$\mathbf{M}_{ff}^i = \int_i \bar{\boldsymbol{\varphi}}^{\mathrm{T}} \bar{\boldsymbol{\varphi}} \mathrm{d}m = \begin{bmatrix} m_{ff}^{11} & m_{ff}^{12} & \cdots & m_{ff}^{1n_f^i} \\ m_{ff}^{21} & m_{ff}^{22} & \cdots & m_{ff}^{2n_f^i} \\ \vdots & \vdots & \vdots & \vdots \\ m_{ff}^{n_f^i 1} & m_{ff}^{n_f^i 2} & \cdots & m_{ff}^{n_f^i n_f^i} \end{bmatrix} \tag{54}$$

$$m_{ff}^{jk} = \int_i \bar{\boldsymbol{\varphi}}_j^{\mathrm{T}} \bar{\boldsymbol{\varphi}}_k \mathrm{d}m = \mathrm{tr}\left(\mathbf{i}_3\left(j,:,:,k\right)\right) \tag{55}$$

3.4 Quadratic-velocity generalized inertia forces.

It is possible to get rid of the time derivative $\dot{\mathbf{M}}$ elaborating on (25b):

$$\mathbf{Q}^v = -\left(\mathbf{M}_{\mathbf{q}} \otimes_3 \dot{\mathbf{q}}\right)\dot{\mathbf{q}} + \frac{1}{2}\left(\mathbf{M}_{\mathbf{q}}^{\mathrm{T}_2} \otimes_2 \dot{\mathbf{q}}\right)\dot{\mathbf{q}} = \left(\left(\frac{1}{2}\left(\mathbf{M}_{\mathbf{q}}\right)^{\mathrm{T}_2} - \mathbf{M}_{\mathbf{q}}\right) \otimes_2 \dot{\mathbf{q}}\right)\dot{\mathbf{q}} \tag{56}$$

Now, the quadratic-velocity generalized inertia forces only depend on the derivatives of the mass matrix with respect to the states, $\mathbf{M}_{\mathbf{q}}$, presented in section 3.4.1. Most of the pieces needed have already been developed in section 3.3, though.

3.4.1 First-order derivatives of the flexible mass matrix w.r.t states

The first derivative of the flexible body mass matrix with respect to the coordinates of the flexible body:

$$(\mathbf{M}_i)_{\mathbf{q}^i} = \begin{bmatrix} \mathbf{M}_{rr} \;\big|_2\; \mathbf{M}_{rf} \\ \mathbf{M}_{rf}^{\mathrm{T}} \;\big|_2\; \mathbf{M}_{ff} \end{bmatrix}_{\mathbf{q}^i} = \begin{bmatrix} (\mathbf{M}_{rr})_{\mathbf{q}^i} \;\big|_2\; (\mathbf{M}_{rf})_{\mathbf{q}^i} \\ (\mathbf{M}_{rf})_{\mathbf{q}^i}^{\mathrm{T}_3} \;\big|_2\; \mathbf{0}_{n_f^i \times n_f^i \times n^i} \end{bmatrix} \tag{57}$$

Block $\left(\mathbf{M}_{rr}^i\right)_{\mathbf{q}^i}$ is the sum of the following contributions.

$$\left(\mathbf{M}_{rr}^i\right)_{\mathbf{q}^i} = \left(\mathbf{M}_{rr2} + \mathbf{M}_{rr2}^{\mathrm{T}}\right)_{\mathbf{q}^i} + (\mathbf{M}_{rr4})_{\mathbf{q}^i} \in \mathbb{R}^{12\times 12\times n^i} \tag{58}$$

$$(\mathbf{M}_{rr2})_{\mathbf{q}^i} = \left[(\mathbf{M}_{rr2})_{\mathbf{q}_r^i} \;\big|_3\; (\mathbf{M}_{rr2})_{\mathbf{q}_f^i}\right] = \left[\mathbf{0}_{12\times 12\times 12} \;\big|_3\; (\mathbf{M}_{rr2})_{\mathbf{q}_f^i}\right] \tag{59}$$

$$(\mathbf{M}_{rr4})_{\mathbf{q}^i} = \left[(\mathbf{M}_{rr4})_{\mathbf{q}_r^i} \;\big|_3\; (\mathbf{M}_{rr4})_{\mathbf{q}_f^i}\right] = \left[\mathbf{0}_{12\times 12\times 12} \;\big|_3\; (\mathbf{M}_{rr4})_{\mathbf{q}_f^i}\right] \tag{60}$$

The sum $\left(\mathbf{M}_{rr2} + \mathbf{M}_{rr2}^{\mathrm{T}}\right)_{\mathbf{q}_f^i}$ can be calculated as a single term:

$$\left(\mathbf{M}_{rr2} + \mathbf{M}_{rr2}^{\mathrm{T}}\right)_{\mathbf{q}_f^i} = \begin{bmatrix} \mathbf{I}_3 \otimes \left(2m_{rr2}^{00}\right)_{\mathbf{q}_f^i} & \big|_2 \mathbf{I}_3 \otimes \left(m_{rr2}^{0k} + m_{rr2}^{k0}\right)_{\mathbf{q}_f^i} \\ \mathbf{I}_3 \otimes \left(m_{rr2}^{j0} + m_{rr2}^{0j}\right)_{\mathbf{q}_f^i} & \big|_2 \mathbf{I}_3 \otimes \left(m_{rr2}^{jk} + m_{rr2}^{kj}\right)_{\mathbf{q}_f^i} \end{bmatrix}; j,k = 1,2,3. \tag{61}$$

where $\left(m_{rr2}^{00}\right)_{\mathbf{q}_f^i}$, $\left(m_{rr2}^{j0}\right)_{\mathbf{q}_f^i}$, $\left(m_{rr2}^{0k}\right)_{\mathbf{q}_f^i}$, $\left(m_{rr2}^{jk}\right)_{\mathbf{q}_f^i}$ are constant terms which have already been used in the construction of the mass matrix (45).

Term $(\mathbf{M}_{rr4})_{\mathbf{q}_f^i}$ is given by:

$$(\mathbf{M}_{rr4})_{\mathbf{q}_f^i} = \begin{bmatrix} \mathbf{I}_3 \otimes \left(m_{rr4}^{00}\right)_{\mathbf{q}_f^i} & \big|_2 & \mathbf{I}_3 \otimes \left(m_{rr4}^{0k}\right)_{\mathbf{q}_f^i} \\ \mathbf{I}_3 \otimes \left(m_{rr4}^{j0}\right)_{\mathbf{q}_f^i} & \big|_2 & \mathbf{I}_3 \otimes \left(m_{rr4}^{jk}\right)_{\mathbf{q}_f^i} \end{bmatrix};\; j,k = 1,2,3. \tag{62}$$

The derivatives in (62) are the derivatives of the elements of $\mathbf{M}_{rr4}^{4\times 4}$ in (50):

$$\left(\mathbf{M}_{rr4}^{4\times 4}\right)_{\mathbf{q}_f^i} = \mathbf{T}_{rr4} \otimes_3 \mathbf{q}_f^i + \mathbf{T}_{rr4} \otimes_4 \mathbf{q}_f^i = \left[\mathbf{T}_{rr4} + \mathbf{T}_{rr4}^{\mathrm{T}_{1,2}}\right] \otimes_4 \mathbf{q}_f^i \tag{63}$$

The last nonzero blocks contributing to $(\mathbf{M}_i)_{\mathbf{q}^i}$ are $(\mathbf{M}_{rf})_{\mathbf{q}^i}$ and $(\mathbf{M}_{fr})_{\mathbf{q}^i}$.

$$(\mathbf{M}_{rf})_{\mathbf{q}^i} = (\mathbf{M}_{rf1})_{\mathbf{q}^i} + (\mathbf{M}_{rf2})_{\mathbf{q}^i} \in \mathbb{R}^{12\times n_f^i \times n^i} \tag{64}$$

$$(\mathbf{M}_{fr})_{\mathbf{q}^i} = \left(\mathbf{M}_{rf}^{\mathrm{T}}\right)_{\mathbf{q}^i} = (\mathbf{M}_{rf})_{\mathbf{q}^i}^{\mathrm{T}_3} \in \mathbb{R}^{n_f^i \times 12\times n^i} \tag{65}$$

$$(\mathbf{M}_{rf1})_{\mathbf{q}^i} = \left[(\mathbf{M}_{rf1})_{\mathbf{q}_r^i} \;\big|_3\; \mathbf{0}_{12\times n_f^i \times n_f^i}\right] = \left[(\mathbf{M}_{rr2})_{\mathbf{q}_f^i}^{\mathrm{T}_1} \;\big|_3\; \mathbf{0}_{12\times n_f^i \times n_f^i}\right] \tag{66}$$

$$(\mathbf{M}_{rf2})_{\mathbf{q}^i} = \left[(\mathbf{M}_{rf2})_{\mathbf{q}_r^i} \big|_3 (\mathbf{M}_{rf2})_{\mathbf{q}_f^i}\right] = \left[(\mathbf{M}_{rf2})_{\mathbf{q}_r^i \mathbf{q}_f^i} \otimes_4 \mathbf{q}_f^i \big|_3 (\mathbf{M}_{rf2})_{\mathbf{q}_r^i \mathbf{q}_f^i} \otimes_3 \mathbf{q}_r^i\right] \tag{67}$$

In (66), the identity $(\mathbf{M}_{rf1})_{\mathbf{q}_r^i} = (\mathbf{M}_{rr2})_{\mathbf{q}_f^i}^{\mathrm{T}_1}$ can be followed from (52a).

3.5 Elastic potential of a flexible body: stiffness matrix

The elastic potential of a flexible body, i, can be expressed by means of the finite element method, using isoparametric elements, as:

$$V^i = \frac{1}{2}\bar{\mathbf{u}}^{*\mathrm{T}}\bar{\mathbf{K}}_i^*\bar{\mathbf{u}}^* \tag{68}$$

where $\bar{\mathbf{u}}^* = \begin{bmatrix}\bar{\mathbf{u}}_1^{*\mathrm{T}} & \bar{\mathbf{u}}_2^{*\mathrm{T}} & \cdots & \bar{\mathbf{u}}_{n_n}^{*\mathrm{T}}\end{bmatrix}^{\mathrm{T}} \in \mathbb{R}^{3n_n}$ are the elastic displacements of the nodes with respect to the undeformed configuration and $\bar{\mathbf{K}}^* \in \mathbb{R}^{3n_n \times 3n_n}$ is the body finite-element stiffness matrix, associated to the nodal displacements with respect to the body floating frame of reference.

The nodal displacements can be approximated by the deformation modes:

$$\bar{\mathbf{u}}^* = \bar{\boldsymbol{\varphi}}^*\mathbf{q}_f^i \tag{69}$$

$$\bar{\boldsymbol{\varphi}}^* = \begin{bmatrix}\bar{\boldsymbol{\varphi}}_1^{*\mathrm{T}} & \bar{\boldsymbol{\varphi}}_2^{*\mathrm{T}} & \dots & \bar{\boldsymbol{\varphi}}_{n_n}^{*\mathrm{T}}\end{bmatrix}^{\mathrm{T}} \in \mathbb{R}^{3n_n \times n_f^i} \tag{70}$$

Replacing in (68):

$$V_i = \frac{1}{2}\mathbf{q}_f^{i\mathrm{T}}\mathbf{K}_{ff}\mathbf{q}_f^i = \frac{1}{2}\mathbf{q}^{i\mathrm{T}}\mathbf{K}_i^e\mathbf{q}^i \tag{71}$$

$$\mathbf{K}_{ff} = \bar{\boldsymbol{\varphi}}^{*\mathrm{T}}\bar{\mathbf{K}}_i^*\bar{\boldsymbol{\varphi}}^* \tag{72}$$

$$\mathbf{K}_i^e = \begin{bmatrix}\mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{K}_{ff}\end{bmatrix} \tag{73}$$

The elastic stiffness matrix of the body, $\mathbf{K}_i^e$, as defined in (73), is constant during the whole simulation. For a specific selection of the deformation modes, simplified expressions can be obtained but, for generality of the approach and code, no further assumptions are taken in the calculation of the elastic stiffness matrix.

In FFR we are dealing with small deformations and we will stick to isotropic materials, resulting in symmetric strain tensors and therefore symmetric finite-element stiffness matrices, $\mathbf{K}^*$. Thus, the symmetry of the stiffness matrix $\mathbf{K}_i^e$ is assumed as well.

4 Sensitivity analysis equations

In this section, the sensitivity analysis of the ALI3-P formulation in section 3 is covered. The formulation is an extension to flexible bodies of those thoroughly described in [13] (direct) and [14, 19] (direct, continuous adjoint and discrete adjoint) for rigid bodies. The final form of the sensitivity equations is as described in the mentioned publications, but there are some new contributions due to the elastic $-\mathbf{K}^e\mathbf{q}$ and velocity dependent forces $\mathbf{Q}^v$ present in equations (25). We will focus on those terms and, for simplicity, we will stick to the direct sensitivity analysis, but the extension of the adjoint needs for the same derivatives and it is straightforward from [14].

The gradient of a set of o objective functions represented by $\boldsymbol{\psi} \in \mathbb{R}^o$ dependent on the states $\mathbf{q}$, $\dot{\mathbf{q}}$ and $\ddot{\mathbf{q}}$, Lagrange multipliers $\boldsymbol{\lambda}^*$ and parameters $\boldsymbol{\rho} \in \mathbb{R}^p$, reads:

$$\boldsymbol{\psi}' = \nabla \boldsymbol{\psi}^{\mathrm{T}} = \frac{\mathrm{d}\boldsymbol{\psi}}{\mathrm{d}\boldsymbol{\rho}} = \int_{t_0}^{t_F} \left(\mathbf{g}_{\mathbf{q}} \mathbf{q}' + \mathbf{g}_{\dot{\mathbf{q}}} \dot{\mathbf{q}}' + \mathbf{g}_{\ddot{\mathbf{q}}} \ddot{\mathbf{q}}' + \mathbf{g}_{\boldsymbol{\lambda}^*} \boldsymbol{\lambda}^{*\prime} + \mathbf{g}_{\boldsymbol{\rho}} \right) \mathrm{d}t \tag{74}$$

According to equation (74), the notation $(\cdot)' = \frac{\mathrm{d}\cdot}{\mathrm{d}\boldsymbol{\rho}}$, profusely used hereafter, means transposed gradients or total derivatives with respect to parameters. Observe that the derivatives of $\mathbf{g}$ can be obtained from the known expression of the objective function, but the terms $\mathbf{q}'$, $\dot{\mathbf{q}}'$, $\ddot{\mathbf{q}}'$ and $\boldsymbol{\lambda}^{*\prime}$ are unknown sensitivity matrices, which must be obtained from the sensitivity analysis of the forward dynamics equations described in section 3.

The new contributions due to the elastic $\mathbf{K}^e\mathbf{q}$ and velocity dependent terms $\mathbf{Q}^v$,

$$\frac{\mathrm{d}\left(\mathbf{K}^e\mathbf{q}\right)}{\mathrm{d}\boldsymbol{\rho}} = \left(\mathbf{K}^e\mathbf{q}\right)' = \mathbf{K}^{e\prime} \otimes_2 \mathbf{q} + \mathbf{K}^e\mathbf{q}' = \mathbf{K}^e\mathbf{q}' + \mathbf{K}^e_{\boldsymbol{\rho}} \otimes_2 \mathbf{q} \tag{75}$$

where $\mathbf{K}^e$ has been assumed constant for each simulation (not dependent on the states), according to section 3.5, but it can depend on some parameters affecting the geometry or material properties of the flexible body, which are constant during each simulation but they can vary in an eventual optimization process.

$$\frac{\mathrm{d}\mathbf{Q}^v}{\mathrm{d}\boldsymbol{\rho}} = \left(\mathbf{Q}^v\right)' = \mathbf{Q}^v_{\dot{\mathbf{q}}}\dot{\mathbf{q}}^{*\prime} + \mathbf{Q}^v_{\mathbf{q}}\mathbf{q}' + \mathbf{Q}^v_{\boldsymbol{\rho}} \tag{76a}$$

$$\mathbf{Q}^v_{\dot{\mathbf{q}}} = \left(\frac{1}{2}\left(\mathbf{M}_{\mathbf{q}}\right)^{\mathrm{T}_2} - \mathbf{M}_{\mathbf{q}}\right) \otimes_2 \dot{\mathbf{q}}^* + \left(\frac{1}{2}\left(\mathbf{M}_{\mathbf{q}}\right)^{\mathrm{T}_2} - \mathbf{M}_{\mathbf{q}}\right) \otimes_3 \dot{\mathbf{q}}^* \tag{76b}$$

$$\mathbf{Q}^v_{\mathbf{q}} = \left[\left(\frac{1}{2}\left(\mathbf{M}_{\mathbf{qq}}\right)^{\mathrm{T}_{2,4}} - \mathbf{M}_{\mathbf{qq}}\right) \otimes_2 \dot{\mathbf{q}}^*\right] \otimes_2 \dot{\mathbf{q}}^* \tag{76c}$$

$$\mathbf{Q}^v_{\boldsymbol{\rho}} = \left[\left(\frac{1}{2}\left(\mathbf{M}_{\mathbf{q}\boldsymbol{\rho}}\right)^{\mathrm{T}_{2,4}} - \mathbf{M}_{\mathbf{q}\boldsymbol{\rho}}\right) \otimes_2 \dot{\mathbf{q}}^*\right] \otimes_2 \dot{\mathbf{q}}^* \tag{76d}$$

Observe that the term $\mathbf{Q}^v_{\mathbf{q}}$ is built with second order derivatives of the mass matrix with respect to the states (described in section (4.4.1)), which are constant for each simulation and thus the sum of the 4-order multidimensional matrices in (76c) can be efficiently evaluated and stored as a preprocess.

Then, the TLM with the rigid body and flexible contributions, reads:

$$\left[\mathbf{M}\ddot{\mathbf{q}}^{*\prime\{i\}} + \bar{\mathbf{C}}\dot{\mathbf{q}}^{*\prime\{i\}} + \bar{\mathbf{K}}\mathbf{q}'^{\{i\}} + \boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}}\boldsymbol{\lambda}^{*\prime\{i\}}\right] = \bar{\mathbf{Q}}^{\boldsymbol{\rho}} \tag{77a}$$

$$\boldsymbol{\lambda}^{*\prime\{i\}} = \boldsymbol{\lambda}^{*\prime\{i-1\}} + \boldsymbol{\alpha}\boldsymbol{\Phi}'^{\{i\}}; \quad i = 0, 1, 2, ..., \tag{77b}$$

$$\boldsymbol{\Phi}'^{\{i\}}_{n+1} = \left(\boldsymbol{\Phi}_{\mathbf{q}}\mathbf{q}'^{\{i\}} + \boldsymbol{\Phi}_{\boldsymbol{\rho}}\right)_{n+1} \tag{77c}$$

$$\bar{\mathbf{K}} = \mathbf{M}_{\mathbf{q}} \otimes_2 \ddot{\mathbf{q}}^* + \boldsymbol{\Phi}^{\mathrm{T}_3}_{\mathbf{qq}} \otimes_2 \left(\boldsymbol{\lambda}^* + \boldsymbol{\alpha}\boldsymbol{\Phi}\right) + \boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}}\boldsymbol{\alpha}\boldsymbol{\Phi}_{\mathbf{q}} + \mathbf{K} + \mathbf{K}^e - \mathbf{Q}^v_{\mathbf{q}} \tag{77d}$$

$$\bar{\mathbf{C}} = \mathbf{C} - \mathbf{Q}^v_{\dot{\mathbf{q}}} \tag{77e}$$

$$\bar{\mathbf{Q}}^{\boldsymbol{\rho}} = \mathbf{Q}_{\boldsymbol{\rho}} - \mathbf{M}_{\boldsymbol{\rho}} \otimes_2 \ddot{\mathbf{q}}^* - \boldsymbol{\Phi}^{\mathrm{T}_3}_{\mathbf{q}\boldsymbol{\rho}} \otimes_2 (\boldsymbol{\lambda}^* + \boldsymbol{\alpha}\boldsymbol{\Phi}) - \boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}}\boldsymbol{\alpha}\boldsymbol{\Phi}_{\boldsymbol{\rho}} - \mathbf{K}^e_{\boldsymbol{\rho}} \otimes_2 \mathbf{q} + \mathbf{Q}^v_{\boldsymbol{\rho}} \tag{77f}$$

where $\mathbf{K} = -\frac{\partial \mathbf{Q}}{\partial \mathbf{q}}$ and $\mathbf{C} = -\frac{\partial \mathbf{Q}}{\partial \dot{\mathbf{q}}}$ are derivatives of the external forces with respect to the states.

Regarding the sensitivities of the projections (26), the same expressions already considered for rigid bodies hold.

$$\begin{aligned}\left[\left(\bar{\mathbf{P}} + \varsigma\boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}}\boldsymbol{\alpha}\boldsymbol{\Phi}_{\mathbf{q}}\right)\dot{\mathbf{q}}'\right]_{n+1} = \Big[&\bar{\mathbf{P}}\dot{\mathbf{q}}^{*\prime} + \bar{\mathbf{P}}' \otimes_2 (\dot{\mathbf{q}}^* - \dot{\mathbf{q}}) - \left(\boldsymbol{\Phi}^{\mathrm{T}_3}_{\mathbf{q}\mathbf{q}} \otimes_2 \varsigma\boldsymbol{\alpha}\dot{\boldsymbol{\Phi}}\right)\mathbf{q}' \\ &- \boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}\boldsymbol{\rho}} \otimes_2 \varsigma\boldsymbol{\alpha}\dot{\boldsymbol{\Phi}} - \boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}}\varsigma\boldsymbol{\alpha}\left(\dot{\boldsymbol{\Phi}}_{\mathbf{q}}\mathbf{q}' + \dot{\boldsymbol{\Phi}}_{\boldsymbol{\rho}}\right)\Big]_{n+1}\end{aligned} \tag{78}$$

$$\begin{aligned}\left[\left(\bar{\mathbf{P}} + \varsigma\boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}}\boldsymbol{\alpha}\boldsymbol{\Phi}_{\mathbf{q}}\right)\ddot{\mathbf{q}}'\right]_{n+1} = \Big[&\bar{\mathbf{P}}\ddot{\mathbf{q}}^{*\prime} + \bar{\mathbf{P}}' \otimes_2 (\ddot{\mathbf{q}}^* - \ddot{\mathbf{q}}) - \left(\boldsymbol{\Phi}^{\mathrm{T}_3}_{\mathbf{q}\mathbf{q}} \otimes_2 \varsigma\boldsymbol{\alpha}\ddot{\boldsymbol{\Phi}}\right)\mathbf{q}' \\ &- \boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}\boldsymbol{\rho}} \otimes_2 \varsigma\boldsymbol{\alpha}\ddot{\boldsymbol{\Phi}} - \boldsymbol{\Phi}^{\mathrm{T}}_{\mathbf{q}}\varsigma\boldsymbol{\alpha}\left(2\dot{\boldsymbol{\Phi}}_{\mathbf{q}}\dot{\mathbf{q}}' + \ddot{\boldsymbol{\Phi}}_{\mathbf{q}}\mathbf{q}' + \ddot{\boldsymbol{\Phi}}_{\boldsymbol{\rho}}\right)\Big]_{n+1}\end{aligned} \tag{79}$$

$$\bar{\mathbf{P}}' \otimes_2 (\dot{\mathbf{q}}^* - \dot{\mathbf{q}}) = \left(\bar{\mathbf{P}}_{\dot{\mathbf{q}}^*} \otimes_2 (\dot{\mathbf{q}}^* - \dot{\mathbf{q}})\right)\dot{\mathbf{q}}^{*\prime} + \left(\bar{\mathbf{P}}_{\mathbf{q}} \otimes_2 (\dot{\mathbf{q}}^* - \dot{\mathbf{q}})\right)\mathbf{q}' + \bar{\mathbf{P}}_{\boldsymbol{\rho}} \otimes_2 (\dot{\mathbf{q}}^* - \dot{\mathbf{q}}) \tag{80}$$

$$\bar{\mathbf{P}}' \otimes_2 (\ddot{\mathbf{q}}^* - \ddot{\mathbf{q}}) = \left(\bar{\mathbf{P}}_{\dot{\mathbf{q}}^*} \otimes_2 (\ddot{\mathbf{q}}^* - \ddot{\mathbf{q}})\right)\dot{\mathbf{q}}^{*\prime} + \left(\bar{\mathbf{P}}_{\mathbf{q}} \otimes_2 (\ddot{\mathbf{q}}^* - \ddot{\mathbf{q}})\right)\mathbf{q}' + \bar{\mathbf{P}}_{\boldsymbol{\rho}} \otimes_2 (\ddot{\mathbf{q}}^* - \ddot{\mathbf{q}}) \tag{81}$$

where the dependencies $\bar{\mathbf{P}} = \bar{\mathbf{P}}(\mathbf{q}, \dot{\mathbf{q}}^*, \boldsymbol{\rho})$ have been assumed.

The multidimensional matrix $\bar{\mathbf{P}}'$ depends on the selection of the projection matrix. For the mass-orthogonal projections $\bar{\mathbf{P}} = \mathbf{M}$, $\bar{\mathbf{P}}_{\dot{\mathbf{q}}} = \mathbf{0}$, $\bar{\mathbf{P}}_{\mathbf{q}} = \mathbf{M}_{\mathbf{q}}$ and $\bar{\mathbf{P}}_{\boldsymbol{\rho}} = \mathbf{M}_{\boldsymbol{\rho}}$.

In the following sections, derivatives of the terms needed for the sensitivity equations (77) are detailed, focusing, mostly, in the specific contributions coming from flexible bodies. For a thorough derivation of the remaining terms also present for rigid bodies and the TLM itself, the reader is referred to the aforementioned publications.

4.1 Derivatives of the flexible body constraints

For the sensitivities coming from the TLM (77), terms $\boldsymbol{\Phi}_{\mathbf{qq}}$, $\boldsymbol{\Phi}_{\mathbf{q}\boldsymbol{\rho}}$ and $\boldsymbol{\Phi}_{\boldsymbol{\rho}}$ are required. From (29):

$$(\boldsymbol{\Phi}_P)_{\mathbf{qq}} = \left[\frac{\partial^2 \boldsymbol{\Phi}_P}{\partial \mathbf{q}^i \partial \mathbf{r}^i_P} \Big|_2 \frac{\partial^2 \boldsymbol{\Phi}_P}{\partial \mathbf{q}^{i2}}\right] = \left[\mathbf{0}_{3\times 3\times n^i} \Big|_2 - \left(\mathbf{L}^i_P\right)_{\mathbf{q}^i}\right] \tag{82}$$

$$\left(\mathbf{L}^i_P\right)_{\mathbf{q}^i} = \left[\left(\mathbf{L}^i_P\right)_{\mathbf{q}^i_r} \Big|_2 \left(\mathbf{L}^i_P\right)_{\mathbf{q}^i_f}\right] \in \mathbb{R}^{3\times n^i \times n^i} \tag{83}$$

$$\left(\mathbf{L}^i_P\right)_{\mathbf{q}^i_r} = \left[\mathbf{0}_{3\times 12\times 12} \Big|_2 (\mathbf{A}_i)_{\mathbf{q}_r} \otimes_2 \bar{\boldsymbol{\varphi}}^i_P\right] \in \mathbb{R}^{3\times n^i \times 12} \tag{84}$$

$$\left(\mathbf{L}^i_P\right)_{\mathbf{q}^i_f} = \left[\left((\mathbf{A}_i)_{\mathbf{q}_r} \otimes_2 \bar{\boldsymbol{\varphi}}^i_P\right)^{\mathrm{T}_1} \Big|_2 \mathbf{0}_{3\times n^i_f \times n_f}\right] \in \mathbb{R}^{3\times n^i \times n^i_f} \tag{85}$$

where $\left(\mathbf{L}^i_P\right)_{\mathbf{q}^i}$ (and therefore $(\boldsymbol{\Phi}_P)_{\mathbf{qq}}$) is constant during the whole simulation.

Concerning the term $(\boldsymbol{\Phi}_P)_{\boldsymbol{\rho}}$, parameters can only be affecting $\mathbf{D}_P$ in equation (28), through the local coordinates of the points or vectors or through the deformation

modes, thus:

$$\left(\boldsymbol{\Phi}_P\right)_{\boldsymbol{\rho}} = -\left(\mathbf{D}_P^i\right)_{\boldsymbol{\rho}} \otimes_2 \mathbf{q}^i \tag{86}$$

$$\left(\mathbf{D}_P^i\right)_{\boldsymbol{\rho}} = \left[\left(\bar{\mathbf{C}}_P\right)_{\boldsymbol{\rho}} \Big|_2 \left(\left(\mathbf{A}_i\right)_{\mathbf{q}_r} \otimes_2 \bar{\boldsymbol{\varphi}}_P^i\right)_{\boldsymbol{\rho}} \otimes_3 \mathbf{q}_r^i\right] \in \mathbb{R}^{3\times n^i\times p} \tag{87}$$

$$\left(\bar{\mathbf{C}}_P\right)_{\boldsymbol{\rho}} = \left[\mathbf{I}_3 \otimes \left(\bar{c}_0^P\right)_{\boldsymbol{\rho}} \Big|_2 \mathbf{I}_3 \otimes \left(\bar{c}_1^P\right)_{\boldsymbol{\rho}} \Big|_2 \mathbf{I}_3 \otimes \left(\bar{c}_2^P\right)_{\boldsymbol{\rho}} \Big|_2 \mathbf{I}_3 \otimes \left(\bar{c}_3^P\right)_{\boldsymbol{\rho}}\right] \tag{88}$$

$$\left(\left(\mathbf{A}_i\right)_{\mathbf{q}_r} \otimes_2 \bar{\boldsymbol{\varphi}}_P^i\right)_{\boldsymbol{\rho}} = \left(\mathbf{A}_i\right)_{\mathbf{q}_r\boldsymbol{\rho}} \otimes_2 \bar{\boldsymbol{\varphi}}_P^i + \left(\left(\mathbf{A}_i\right)_{\mathbf{q}_r} \otimes_2 \left(\bar{\boldsymbol{\varphi}}_P^i\right)_{\boldsymbol{\rho}}\right)^{\mathrm{T}_{1,2}} \tag{89}$$

$$\left(\mathbf{A}_i\right)_{\mathbf{q}_r\boldsymbol{\rho}} = \left(\left(\mathbf{X}_i\right)_{\mathbf{q}_r} \otimes_2 \left(\bar{\mathbf{X}}_i^{-1}\right)_{\boldsymbol{\rho}}\right)^{\mathrm{T}_{1,2}} \tag{90}$$

$$\left(\bar{\mathbf{X}}_i^{-1}\right)_{\boldsymbol{\rho}} = -\bar{\mathbf{X}}_i^{-1}\left(\bar{\mathbf{X}}_i\right)_{\boldsymbol{\rho}}\bar{\mathbf{X}}_i^{-1} \tag{91}$$

$$\left(\bar{\mathbf{X}}_i\right)_{\boldsymbol{\rho}} = \left(\bar{\mathbf{X}}_3^i\right)_{\boldsymbol{\rho}} + \left[\left(\bar{\mathbf{r}}_0^i\right)_{\boldsymbol{\rho}} \otimes \mathbf{b}^{\mathrm{T}}\right]^{\mathrm{T}_1} \tag{92}$$

with the derivatives of the coefficients $\bar{\mathbf{c}}_P = \left[\bar{c}_0^P \;\; \bar{\mathbf{c}}_P^3\right]^{\mathrm{T}} = \left[\bar{c}_0^P \;\; \bar{c}_1^P \;\; \bar{c}_2^P \;\; \bar{c}_3^P\right]^{\mathrm{T}}$,

$$\left(\bar{\mathbf{c}}_P\right)_{\boldsymbol{\rho}} = \begin{bmatrix}\left(\bar{c}_0^P\right)_{\boldsymbol{\rho}} \\ \left(\bar{\mathbf{c}}_P^3\right)_{\boldsymbol{\rho}}\end{bmatrix} = \begin{bmatrix}\mathbf{b}_i^{\mathrm{T}}\left(\bar{\mathbf{c}}_P^3\right)_{\boldsymbol{\rho}} \\ \left(\bar{\mathbf{X}}_i^{-1}\right)_{\boldsymbol{\rho}} \otimes_2 \left(\bar{\mathbf{r}}_{r,P}^i - b_0^P\bar{\mathbf{r}}_0^i\right) + \bar{\mathbf{X}}_i^{-1}\left(\left(\bar{\mathbf{r}}_{r,P}^i\right)_{\boldsymbol{\rho}} - b_0^P\left(\bar{\mathbf{r}}_0^i\right)_{\boldsymbol{\rho}}\right)\end{bmatrix} \tag{93}$$

Term $\left(\boldsymbol{\Phi}_P\right)_{\mathbf{q}}$ could depend on the parameters $\boldsymbol{\rho}$, then:

$$\left(\boldsymbol{\Phi}_P\right)_{\mathbf{q}\boldsymbol{\rho}} = \left[\frac{\partial^2\boldsymbol{\Phi}_P}{\partial\boldsymbol{\rho}\partial\mathbf{r}_P^i} \Big|_2 \frac{\partial^2\boldsymbol{\Phi}_P}{\partial\boldsymbol{\rho}\partial\mathbf{q}}\right] = \left[\mathbf{0}_{3\times3\times p} \Big|_2 -\left(\mathbf{L}_P^i\right)_{\boldsymbol{\rho}}\right] \tag{94}$$

$$\left(\mathbf{L}_P^i\right)_{\boldsymbol{\rho}} = \left[\left(\bar{\mathbf{C}}_P\right)_{\boldsymbol{\rho}} + \left(\left(\mathbf{A}_i\right)_{\mathbf{q}_r} \otimes_2 \bar{\boldsymbol{\varphi}}_P^i\right)_{\boldsymbol{\rho}} \otimes_2 \mathbf{q}_f^i \Big|_2 \left(\left(\mathbf{A}_i\right)_{\mathbf{q}_r} \otimes_2 \bar{\boldsymbol{\varphi}}_P^i\right)_{\boldsymbol{\rho}} \otimes_3 \mathbf{q}_r^i\right] \in \mathbb{R}^{3\times n^i\times p} \tag{95}$$

For equation (78), the term $\dot{\boldsymbol{\Phi}}_{\boldsymbol{\rho}}$ is needed.

$$\dot{\boldsymbol{\Phi}}_P = \dot{\mathbf{r}}_P^i - \dot{\mathbf{r}}_{r,P}^i - \dot{\mathbf{r}}_{f,P}^i = \dot{\mathbf{r}}_P^i - \mathbf{L}_P^i\dot{\mathbf{q}}^i \Rightarrow \left(\dot{\boldsymbol{\Phi}}_P\right)_{\boldsymbol{\rho}} = -\left(\mathbf{L}_P^i\right)_{\boldsymbol{\rho}} \otimes_2 \dot{\mathbf{q}}^i \tag{96}$$

and for equation (79), $\ddot{\boldsymbol{\Phi}}_{\mathbf{q}}$ and $\ddot{\boldsymbol{\Phi}}_{\boldsymbol{\rho}}$ can be obtained from:

$$\ddot{\boldsymbol{\Phi}}_{\mathbf{q}} = \boldsymbol{\Phi}_{\mathbf{qq}} \otimes_2 \ddot{\mathbf{q}} + \dot{\boldsymbol{\Phi}}_{\mathbf{qq}} \otimes_2 \dot{\mathbf{q}} + \dot{\boldsymbol{\Phi}}_{t\mathbf{q}} \tag{97}$$

$$\ddot{\boldsymbol{\Phi}}_{\boldsymbol{\rho}} = \boldsymbol{\Phi}_{\mathbf{q}\boldsymbol{\rho}} \otimes_2 \ddot{\mathbf{q}} + \dot{\boldsymbol{\Phi}}_{\mathbf{q}\boldsymbol{\rho}} \otimes_2 \dot{\mathbf{q}} + \dot{\boldsymbol{\Phi}}_{t\boldsymbol{\rho}} \tag{98}$$

Terms $\dot{\boldsymbol{\Phi}}_{t\mathbf{q}}$, $\dot{\boldsymbol{\Phi}}_{t\boldsymbol{\rho}}$ vanish for scleronomic constraints (and they are case-dependent otherwise), $\boldsymbol{\Phi}_{\mathbf{qq}}$, $\boldsymbol{\Phi}_{\mathbf{q}\boldsymbol{\rho}}$ are given by equations (82), (94), $\dot{\boldsymbol{\Phi}}_{\mathbf{qq}} = \left(\dot{\boldsymbol{\Phi}}_{\mathbf{q}}\right)_{\mathbf{q}} = \mathbf{0}$ and

$\dot{\mathbf{\Phi}}_{\mathbf{q}\boldsymbol{\rho}} = \left(\dot{\mathbf{\Phi}}_{\mathbf{q}}\right)_{\boldsymbol{\rho}}$ [5] is formed by:

$$\left(\dot{\mathbf{\Phi}}_P\right)_{\mathbf{q}\boldsymbol{\rho}} = \left[\frac{\partial^2 \dot{\mathbf{\Phi}}_P}{\partial \boldsymbol{\rho} \partial \mathbf{r}_P^i} \Big|_2 \frac{\partial^2 \dot{\mathbf{\Phi}}_P}{\partial \boldsymbol{\rho} \partial \mathbf{q}}\right] = \left[\mathbf{0}_{3\times 3\times p} \Big|_2 - \left(\dot{\mathbf{L}}_P^i\right)_{\boldsymbol{\rho}}\right] \tag{99}$$

$$\left(\dot{\mathbf{L}}_P^i\right)_{\boldsymbol{\rho}} = \left[\left(\left(\mathbf{A}_i\right)_{\mathbf{q}_r} \otimes_2 \bar{\boldsymbol{\varphi}}_P^i\right)_{\boldsymbol{\rho}} \otimes_2 \dot{\mathbf{q}}_f^i \Big|_2 \left(\left(\mathbf{A}_i\right)_{\mathbf{q}_r} \otimes_2 \bar{\boldsymbol{\varphi}}_P^i\right)_{\boldsymbol{\rho}} \otimes_3 \dot{\mathbf{q}}_r^i\right] \in \mathbb{R}^{3\times n^i \times p} \tag{100}$$

4.2 Derivatives of elastic forces.

Elastic forces, as described in section 3.5, can be modeled as the product of a constant elastic stiffness matrix times the coordinates of the system. The elastic stiffness matrix, however, depends on the geometry of the body and therefore on any parameter affecting it. Considering that a modification of the shape of the body might alter both the deformation modes and the finite element stiffness matrix, the stiffness matrix derivative can be expressed as:

$$\left(\mathbf{K}_i^e\right)_{\boldsymbol{\rho}} = \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \left(\mathbf{K}_{ff}\right)_{\boldsymbol{\rho}} \end{bmatrix} \tag{101}$$

$$\left(\mathbf{K}_{ff}\right)_{\boldsymbol{\rho}} = \left(\bar{\boldsymbol{\varphi}}^{*\mathrm{T}}\right)_{\boldsymbol{\rho}} \otimes_2 \left(\mathbf{K}_i^* \bar{\boldsymbol{\varphi}}^*\right) + \bar{\boldsymbol{\varphi}}^{*\mathrm{T}} \left(\mathbf{K}_i^*\right)_{\boldsymbol{\rho}} \otimes_2 \bar{\boldsymbol{\varphi}}^* + \bar{\boldsymbol{\varphi}}^{*\mathrm{T}} \mathbf{K}_i^* \left(\bar{\boldsymbol{\varphi}}^*\right)_{\boldsymbol{\rho}} \tag{102}$$

4.3 Derivatives of external and gravity forces.

The derivatives of the external forces with respect to the states and parameters, result in several contributions: $\mathbf{K} = -\frac{\partial \mathbf{Q}}{\partial \mathbf{q}}$, is part of the total equivalent stiffness matrix, $\bar{\mathbf{K}}$ in (77d); $\mathbf{C} = -\frac{\partial \mathbf{Q}}{\partial \dot{\mathbf{q}}}$ is needed for the equivalent damping matrix, $\bar{\mathbf{C}}$ in (77d); $\mathbf{Q}_{\boldsymbol{\rho}}$ gathers all the derivatives of the external forces with respect to parameters, required for the right-hand side of the TLM, $\bar{\mathbf{Q}}^{\boldsymbol{\rho}}$ (eq. (77f)).

The contribution of an external force applied on a point of a flexible body, given by equation (31), to the equivalent stiffness matrix of the external forces, $\mathbf{K}$, is given by:

$$\mathbf{K}_{F,P} = -\frac{\partial \left(\mathbf{L}_P^{i\mathrm{T}} \mathbf{F}\right)}{\partial \mathbf{q}} = -\mathbf{F}^{\mathrm{T}} \left(\mathbf{L}_P^i\right)_{\mathbf{q}} - \mathbf{L}_P^{i\mathrm{T}} \mathbf{F}_{\mathbf{q}} \tag{103}$$

$$\left(\mathbf{Q}_{F,P}\right)_{\boldsymbol{\rho}} = \frac{\partial \left(\mathbf{L}_P^{i\mathrm{T}} \mathbf{F}\right)}{\partial \boldsymbol{\rho}} = \mathbf{F}^{\mathrm{T}} \left(\mathbf{L}_P^i\right)_{\boldsymbol{\rho}} + \mathbf{L}_P^{i\mathrm{T}} \mathbf{F}_{\boldsymbol{\rho}} \tag{104}$$

$$\mathbf{C}_{F,P} = -\frac{\partial \left(\mathbf{L}_P^{i\mathrm{T}} \mathbf{F}\right)}{\partial \dot{\mathbf{q}}} = -\mathbf{L}_P^{i\mathrm{T}} \mathbf{F}_{\dot{\mathbf{q}}} \tag{105}$$

where $\left(\mathbf{L}_P^i\right)_{\mathbf{q}}$ is given by equation (83). Because $\left(\mathbf{L}_P^i\right)_{\mathbf{q}^i}$ is a symmetric third order matrix with respect to dimensions 1 and 3 (i.e. $\left(\mathbf{L}_P^i\right)_{\mathbf{q}^i}^{\mathrm{T}_1} = \left(\mathbf{L}_P^i\right)_{\mathbf{q}^i}$) then $\mathbf{F}^{\mathrm{T}} \left(\mathbf{L}_P^i\right)_{\mathbf{q}}$ is a symmetric matrix and $\mathbf{K}_{F,P}$ is also symmetric if $\mathbf{L}_P^{i\mathrm{T}} \mathbf{F}_{\mathbf{q}}$ is symmetric. For general forces, symmetry cannot be assumed (neither for $\mathbf{C}_{F,P}$) and this is relevant for the linear algebra required in the computations and resolution of linear systems.

[5] In this case, the relation $\dot{\mathbf{\Phi}}_{\mathbf{q}} = \frac{\mathrm{d}\mathbf{\Phi}_{\mathbf{q}}}{\mathrm{d}t} = \frac{\partial \dot{\mathbf{\Phi}}}{\partial \mathbf{q}}$ holds.

Concerning gravity forces, $\mathbf{K}_g^i = -\dfrac{\partial \mathbf{Q}_g^i}{\partial \mathbf{q}^i}$ has already been defined in (33) and:

$$\left(\mathbf{Q}_g^i\right)_{\boldsymbol{\rho}} = \begin{bmatrix} \left(\mathbf{Q}_{r,g}^i\right)_{\boldsymbol{\rho}} \\ \mathbf{0}_{n_f^i \times p} \end{bmatrix} - \left(\mathbf{K}_g^i\right)_{\boldsymbol{\rho}} \otimes_2 \mathbf{q}^i \tag{106a}$$

$$\left(\mathbf{Q}_{r,g}^i\right)_{\boldsymbol{\rho}} = \bar{\mathbf{C}}_G^{\mathrm{T}} \mathbf{g} \otimes \left(m_i\right)_{\boldsymbol{\rho}} + m_i \left(\bar{\mathbf{C}}_G^{\mathrm{T}}\right)_{\boldsymbol{\rho}} \otimes_2 \mathbf{g} \tag{106b}$$

$$\left(\mathbf{K}_g^i\right)_{\boldsymbol{\rho}} = -\begin{bmatrix} \mathbf{0}_{12\times 12\times p} & \big|_2 & \left[\mathbf{g}^{\mathrm{T}} \left(\left(\mathbf{X}_i\right)_{\mathbf{q}_r^i} \otimes_2 \mathbf{i}_1^{\bar{\mathbf{X}}_i}\right)_{\boldsymbol{\rho}}\right]^{\mathrm{T}_3} \\ \mathbf{g}^{\mathrm{T}} \left(\left(\mathbf{X}_i\right)_{\mathbf{q}_r^i} \otimes_2 \mathbf{i}_1^{\bar{\mathbf{X}}_i}\right)_{\boldsymbol{\rho}} & \big|_2 & \mathbf{0}_{n_f^i \times n_f^i \times p} \end{bmatrix} \tag{106c}$$

with the gravity assumed to be a non-parameter and

$$\left(\left(\mathbf{X}_i\right)_{\mathbf{q}_r^i} \otimes_2 \mathbf{i}_1^{\bar{\mathbf{X}}_i}\right)_{\boldsymbol{\rho}} = \left(\mathbf{X}_i\right)_{\mathbf{q}_r^i \boldsymbol{\rho}} \otimes_2 \mathbf{i}_1^{\bar{\mathbf{X}}_i} + \left(\left(\mathbf{X}_i\right)_{\mathbf{q}_r^i} \otimes_2 \left(\mathbf{i}_1^{\bar{\mathbf{X}}_i}\right)_{\boldsymbol{\rho}}\right)^{\mathrm{T}_{1,2}} \tag{107}$$

$$\left(m_i\right)_{\boldsymbol{\rho}} = \int_{\partial i} \mathrm{d}m \tag{108}$$

$$\left(\bar{\mathbf{r}}_{r,G}^i\right)_{\boldsymbol{\rho}} = -\frac{1}{m_i} \bar{\mathbf{r}}_{r,G}^i \otimes \left(m_i\right)_{\boldsymbol{\rho}} + \frac{1}{m_i} \int_{\partial i} \mathbf{r}_r \mathrm{d}m \tag{109}$$

$$\left(\mathbf{i}_1^{\bar{\mathbf{X}}_i}\right)_{\boldsymbol{\rho}} = \left(\bar{\mathbf{X}}_i^{-1}\right)_{\boldsymbol{\rho}} \otimes_2 \mathbf{i}_1^i + \bar{\mathbf{X}}_i^{-1} \left(\mathbf{i}_1^i\right)_{\boldsymbol{\rho}} \tag{110}$$

$$\left(\mathbf{i}_1^i\right)_{\boldsymbol{\rho}} = \int_i \bar{\boldsymbol{\varphi}}_{\boldsymbol{\rho}} \mathrm{d}m + \int_{\partial i} \bar{\boldsymbol{\varphi}} \mathrm{d}m \tag{111}$$

The variation ∂i in the limits of integrals (108) and (111) means that the magnitudes may depend on parameters affecting the geometry of the flexible body and the variation of them with the geometry must be taken into account. Integral $\left(\mathbf{i}_1^i\right)_{\boldsymbol{\rho}}$ is constant while the parameters (geometry or material) of the flexible body do not change, therefore, multidimensional matrix $\left(\mathbf{i}_1^{\bar{\mathbf{X}}_i}\right)_{\boldsymbol{\rho}} \in \mathbb{R}^{3\times n_f^i \times p}$ is constant, at least, during each whole simulation.

4.4 Derivatives of the flexible mass matrix

The mass matrix involves a number of derivatives for the computation of sensitivities. They can be divided in derivatives with respect to the states and derivatives with respect to parameters. The first order derivatives with respect to the states have already been obtained in section 3.4.1 because they are needed for the dynamics. The rest of derivatives needed for sensitivities are depicted here.

4.4.1 Second-order derivatives of the flexible mass matrix w.r.t states

The second order derivative of the flexible body mass matrix with respect to the coordinates of the flexible body is represented as a fourth order multidimensional

matrix:

$$(\mathbf{M}_i)_{\mathbf{q}^i\mathbf{q}^i} = \begin{bmatrix} (\mathbf{M}_{rr})_{\mathbf{q}^i\mathbf{q}^i}\big|_2 & (\mathbf{M}_{rf})_{\mathbf{q}^i\mathbf{q}^i} \\ (\mathbf{M}_{rf})^{\mathrm{T}_{3,4}}_{\mathbf{q}^i\mathbf{q}^i}\big|_2 \mathbf{0}_{n_f^i\times n_f^i\times n^i\times n^i} \end{bmatrix} \in \mathbb{R}^{n^i\times n^i\times n^i\times n^i} \tag{112}$$

Most of the terms composing the flexible mass matrix are constant or linear with the states $\mathbf{q}^i$ and they do not contribute to the second derivative. The only contribution in the first block $(\mathbf{M}_{rr})$ comes from $(\mathbf{M}_{rr4})$ which is bilinear with the flexible states $\mathbf{q}_f$, resulting in the following constant second-order derivative.

$$(\mathbf{M}_{rr})_{\mathbf{q}_f^i\mathbf{q}_f^i} = (\mathbf{M}_{rr4})_{\mathbf{q}_f^i\mathbf{q}_f^i} = \begin{bmatrix} \mathbf{I}_3\otimes\left(m^{00}_{rr4}\right)_{\mathbf{q}_f^i\mathbf{q}_f^i} & \mathbf{I}_3\otimes\left(m^{0k}_{rr4}\right)_{\mathbf{q}_f^i\mathbf{q}_f^i} \\ \mathbf{I}_3\otimes\left(m^{j0}_{rr4}\right)_{\mathbf{q}_f^i\mathbf{q}_f^i} & \mathbf{I}_3\otimes\left(m^{jk}_{rr4}\right)_{\mathbf{q}_f^i\mathbf{q}_f^i} \end{bmatrix};\ j,k=1,2,3. \tag{113}$$

The derivatives in (113) are the elements of (50b) and the derivative of the full expression (63) can easily be obtained as well:

$$\left(\mathbf{M}^{4\times4}_{rr4}\right)_{\mathbf{q}_f^i\mathbf{q}_f^i} = \mathbf{T}_{rr4} + \mathbf{T}^{\mathrm{T}_{1,2}}_{rr4} \tag{114}$$

The second block $\mathbf{M}_{rf}$ is composed of the linear term $\mathbf{M}_{rf1}$, not contributing to the second derivative, and the bilinear term $\mathbf{M}_{rf2}$ with the following contribution:

$$\begin{aligned}(\mathbf{M}_{rf2})_{\mathbf{q}^i\mathbf{q}^i} &= \left\{ \left[(\mathbf{M}_{rf2})_{\mathbf{q}_r^i}\big|_3 (\mathbf{M}_{rf2})_{\mathbf{q}_f^i}\right]_{\mathbf{q}_r^i} \middle|_4 \left[(\mathbf{M}_{rf2})_{\mathbf{q}_r^i}\big|_3 (\mathbf{M}_{rf2})_{\mathbf{q}_f^i}\right]_{\mathbf{q}_f^i} \right\} = \\ &= \left\{ \left[\mathbf{0}_{12\times n_f^i\times 12\times 12}\big|_3 (\mathbf{M}_{rf2})^{\mathrm{T}_{1,2}}_{\mathbf{q}_r^i\mathbf{q}_f^i}\right] \middle|_4 \left[(\mathbf{M}_{rf2})_{\mathbf{q}_r^i\mathbf{q}_f^i}\big|_3 \mathbf{0}_{12\times n_f^i\times n_f^i\times n_f^i}\right] \right\}\end{aligned} \tag{115}$$

Clairaut's symmetry of the second derivatives has been used for equation (115), $(\mathbf{M}_{rf2})_{\mathbf{q}_f^i\mathbf{q}_r^i} = (\mathbf{M}_{rf2})^{\mathrm{T}_{1,2}}_{\mathbf{q}_r^i\mathbf{q}_f^i}$ and $(\mathbf{M}_{rf2})_{\mathbf{q}_r^i\mathbf{q}_f^i}$ has already been defined in (53b).

4.5 Derivatives of the flexible mass matrix w.r.t parameters.

According to (77f) and (76d), the derivatives $\mathbf{M}_{\boldsymbol{\rho}}$ and $\mathbf{M}_{\mathbf{q}\boldsymbol{\rho}}$ are needed for the term $\bar{\mathbf{Q}}^{\boldsymbol{\rho}}$ in (77). A parameter that affects the geometry of a flexible body in its undeformed configuration has an impact on the shape integrals needed for the mass matrix, i.e. m_i, $\bar{\boldsymbol{r}}^i_{G,r}$, $\bar{\mathbf{P}}^i_0$, $\mathbf{i}^i_1$, $\mathbf{i}^i_2$ and $\mathbf{i}^i_3$. Therefore, it is necessary to determine their partial derivatives with respect to them for a sensitivity analysis of the dynamics. The mass matrix of a flexible body is also affected by the coordinates of the points and vectors used to describe its rigid body motion.

For the elemental mass matrix, of body i:

$$(\mathbf{M}_i)_{\boldsymbol{\rho}} = \begin{bmatrix} (\mathbf{M}_{rr})_{\boldsymbol{\rho}}\big|_2 (\mathbf{M}_{rf})_{\boldsymbol{\rho}} \\ (\mathbf{M}_{fr})_{\boldsymbol{\rho}}\big|_2 (\mathbf{M}_{ff})_{\boldsymbol{\rho}} \end{bmatrix} = \begin{bmatrix} (\mathbf{M}_{rr})_{\boldsymbol{\rho}}\big|_2 (\mathbf{M}_{rf})_{\boldsymbol{\rho}} \\ (\mathbf{M}_{rf})^{\mathrm{T}_3}_{\boldsymbol{\rho}}\big|_2 (\mathbf{M}_{ff})_{\boldsymbol{\rho}} \end{bmatrix} \in \mathbb{R}^{n^i\times n^i\times p} \tag{116}$$

$$(\mathbf{M}_i)_{\mathbf{q}^i\boldsymbol{\rho}} = \begin{bmatrix} (\mathbf{M}_{rr})_{\mathbf{q}^i\boldsymbol{\rho}}\big|_2 (\mathbf{M}_{rf})_{\mathbf{q}^i\boldsymbol{\rho}} \\ (\mathbf{M}_{fr})_{\mathbf{q}^i\boldsymbol{\rho}}\big|_2 \mathbf{0}_{n_f^i\times n_f^i\times n^i\times p} \end{bmatrix} = \begin{bmatrix} (\mathbf{M}_{rr})_{\mathbf{q}^i\boldsymbol{\rho}}\big|_2 (\mathbf{M}_{rf})_{\mathbf{q}^i\boldsymbol{\rho}} \\ (\mathbf{M}_{rf})^{\mathrm{T}_{3,4}}_{\mathbf{q}^i\boldsymbol{\rho}}\big|_2 \mathbf{0}_{n_f^i\times n_f^i\times n^i\times p} \end{bmatrix} \in \mathbb{R}^{n^i\times n^i\times n^i\times p} \tag{117}$$

with,

$$\left(\mathbf{M}_{rr}\right)_{\boldsymbol{\rho}} = \left(\mathbf{M}_{rr1}\right)_{\boldsymbol{\rho}} + \left(\mathbf{M}_{rr2} + \mathbf{M}_{rr2}^{\mathrm{T}}\right)_{\boldsymbol{\rho}} + \left(\mathbf{M}_{rr4}\right)_{\boldsymbol{\rho}} \in \mathbb{R}^{12\times 12\times p} \tag{118}$$

$$\left(\mathbf{M}_{rf}\right)_{\boldsymbol{\rho}} = \left(\mathbf{M}_{rf1}\right)_{\boldsymbol{\rho}} + \left(\mathbf{M}_{rf2}\right)_{\boldsymbol{\rho}} \in \mathbb{R}^{12\times n_f^i\times p} \tag{119}$$

$$\left(\mathbf{M}_{rf}\right)_{\mathbf{q}^i\boldsymbol{\rho}} = \left(\mathbf{M}_{rf1}\right)_{\mathbf{q}^i\boldsymbol{\rho}} + \left(\mathbf{M}_{rf2}\right)_{\mathbf{q}^i\boldsymbol{\rho}} \in \mathbb{R}^{12\times n_f^i\times n^i\times p} \tag{120}$$

$$\left(\mathbf{M}_{rr}\right)_{\mathbf{q}^i\boldsymbol{\rho}} = \left(\mathbf{M}_{rr2} + \mathbf{M}_{rr2}^{\mathrm{T}}\right)_{\mathbf{q}^i\boldsymbol{\rho}} + \left(\mathbf{M}_{rr4}\right)_{\mathbf{q}^i\boldsymbol{\rho}} \in \mathbb{R}^{12\times 12\times n^i\times p} \tag{121}$$

Where, $\left(\mathbf{M}_{rr1}\right)_{\boldsymbol{\rho}}$ is built with the following derivatives of the 4×4 matrix:

$$\left(\mathbf{M}_{rr1}^{4\times 4}\right)_{\boldsymbol{\rho}} = \int_i \begin{bmatrix} \bar{c}_0^2 & \bar{c}_0\bar{\mathbf{c}}^{3\mathrm{T}} \\ \bar{\mathbf{c}}^3\bar{c}_0 & \bar{\mathbf{c}}^3\otimes\bar{\mathbf{c}}^3 \end{bmatrix}_{\boldsymbol{\rho}} \mathrm{d}m = \int_i \begin{bmatrix} \left(\bar{c}_0^2\right)_{\boldsymbol{\rho}} & \left(\bar{\mathbf{c}}^3\bar{c}_0\right)_{\boldsymbol{\rho}}^{\mathrm{T}_3} \\ \left(\bar{\mathbf{c}}^3\bar{c}_0\right)_{\boldsymbol{\rho}} & \left(\bar{\mathbf{c}}^3\otimes\bar{\mathbf{c}}^3\right)_{\boldsymbol{\rho}} \end{bmatrix}_2 \mathrm{d}m \tag{122}$$

$$\begin{aligned}\int_i \left(\bar{c}_0^2\right)_{\boldsymbol{\rho}} \mathrm{d}m = \left(1 + 2\mathbf{b}_i^{\mathrm{T}}\bar{\mathbf{X}}_i^{-1}\left(\bar{\mathbf{r}}_{r,G}^i - \bar{\mathbf{r}}_0^i\right)\right)\otimes\left(m_i\right)_{\boldsymbol{\rho}} + \mathbf{b}_i^{\mathrm{T}}\left(\bar{\mathbf{X}}_i^{-1}\bar{\mathbf{P}}_0^i\bar{\mathbf{X}}_i^{-\mathrm{T}}\right)_{\boldsymbol{\rho}}\otimes_2\mathbf{b}_i + \\ +2m_i\mathbf{b}_i^{\mathrm{T}}\left[\bar{\mathbf{X}}_i^{-1}\left(\bar{\mathbf{r}}_{r,G}^i - \bar{\mathbf{r}}_0^i\right)\right]_{\boldsymbol{\rho}}\end{aligned} \tag{123}$$

$$\int_i \left(\bar{\mathbf{c}}^3\bar{c}_0\right)_{\boldsymbol{\rho}} \mathrm{d}m = m_i\left[\bar{\mathbf{X}}_i^{-1}\left(\bar{\mathbf{r}}_{r,G}^i - \bar{\mathbf{r}}_0^i\right)\right]_{\boldsymbol{\rho}} + \left(\bar{\mathbf{X}}_i^{-1}\bar{\mathbf{P}}_0^i\bar{\mathbf{X}}_i^{-\mathrm{T}}\right)_{\boldsymbol{\rho}}\otimes_2\mathbf{b}_i \tag{124}$$

$$\int_i \bar{\mathbf{c}}^3\otimes\bar{\mathbf{c}}^3\mathrm{d}m = \left(\bar{\mathbf{X}}_i^{-1}\bar{\mathbf{P}}_0^i\bar{\mathbf{X}}_i^{-\mathrm{T}}\right)_{\boldsymbol{\rho}} \tag{125}$$

with extra dimensions of size 1 assumed for $\left(\bar{\mathbf{c}}^3\bar{c}_0\right)_{\boldsymbol{\rho}} \in \mathbb{R}^{3\times 1\times p}$ and $\left(\bar{c}_0^2\right)_{\boldsymbol{\rho}} \in \mathbb{R}^{1\times 1\times p}$,

$$\left[\bar{\mathbf{X}}_i^{-1}\left(\bar{\mathbf{r}}_{r,G}^i - \bar{\mathbf{r}}_0^i\right)\right]_{\boldsymbol{\rho}} = \left(\bar{\mathbf{X}}_i^{-1}\right)_{\boldsymbol{\rho}}\otimes_2\left(\bar{\mathbf{r}}_{r,G}^i - \bar{\mathbf{r}}_0^i\right) + \bar{\mathbf{X}}_i^{-1}\left(\left(\bar{\mathbf{r}}_{r,G}^i\right)_{\boldsymbol{\rho}} - \left(\bar{\mathbf{r}}_0^i\right)_{\boldsymbol{\rho}}\right) \tag{126}$$

$$\begin{aligned}\left(\bar{\mathbf{X}}_i^{-1}\bar{\mathbf{P}}_0^i\bar{\mathbf{X}}_i^{-\mathrm{T}}\right)_{\boldsymbol{\rho}} = \left(\bar{\mathbf{X}}_i^{-1}\right)_{\boldsymbol{\rho}}\otimes_2\bar{\mathbf{P}}_0^i\bar{\mathbf{X}}_i^{-\mathrm{T}} + \bar{\mathbf{X}}_i^{-1}\left(\bar{\mathbf{P}}_0^i\right)_{\boldsymbol{\rho}}\otimes_2\bar{\mathbf{X}}_i^{-\mathrm{T}} + \\ +\bar{\mathbf{X}}_i^{-1}\bar{\mathbf{P}}_0^i\left(\bar{\mathbf{X}}_i^{-1}\right)_{\boldsymbol{\rho}}^{\mathrm{T}_3}\end{aligned} \tag{127}$$

$$\begin{aligned}\left(\bar{\mathbf{P}}_0^i\right)_{\boldsymbol{\rho}} = -\int_i\left[\left(\left(\bar{\mathbf{r}}_0\right)_{\boldsymbol{\rho}}\otimes\left(\bar{\mathbf{r}}_r - \bar{\mathbf{r}}_0\right)\right)^{\mathrm{T}_1} + \left(\bar{\mathbf{r}}_r - \bar{\mathbf{r}}_0\right)\otimes\left(\bar{\mathbf{r}}_0\right)_{\boldsymbol{\rho}}\right]\mathrm{d}m + \\ +\int_{\partial i}\left(\bar{\mathbf{r}}_r - \bar{\mathbf{r}}_0\right)\left(\bar{\mathbf{r}}_r - \bar{\mathbf{r}}_0\right)^{\mathrm{T}}\mathrm{d}m\end{aligned} \tag{128}$$

Similarly, $\left(\mathbf{M}_{rr2}\right)_{\boldsymbol{\rho}}$, $\left(\mathbf{M}_{rr2}\right)_{\mathbf{q}^i\boldsymbol{\rho}}$, $\left(\mathbf{M}_{rf1}\right)_{\boldsymbol{\rho}}$ and $\left(\mathbf{M}_{rf1}\right)_{\mathbf{q}^i\boldsymbol{\rho}}$ are built with the following derivatives:

$$\left(\mathbf{M}_{rr2}^{4\times 4}\right)_{\boldsymbol{\rho}} = \begin{bmatrix} m_{rr2}^{\mathbf{00}} & \left(\mathbf{m}_{rr2}^{\mathbf{30}}\right)^{\mathrm{T}} \\ \left(\mathbf{m}_{rr2}^{\mathbf{03}}\right)^{\mathrm{T}} & \left(\mathbf{M}_{rr2}^{\mathbf{33}}\right)^{\mathrm{T}} \end{bmatrix}_{\boldsymbol{\rho}} = \begin{bmatrix} \left(m_{rr2}^{\mathbf{00}}\right)_{\boldsymbol{\rho}} & \left(\mathbf{m}_{rr2}^{\mathbf{30}}\right)_{\boldsymbol{\rho}}^{\mathrm{T}_3} \\ \left(\mathbf{m}_{rr2}^{\mathbf{03}}\right)_{\boldsymbol{\rho}}^{\mathrm{T}_3} & \left(\mathbf{M}_{rr2}^{\mathbf{33}}\right)_{\boldsymbol{\rho}}^{\mathrm{T}_3} \end{bmatrix}_2 \tag{129a}$$

$$\left(\mathbf{m}_{rr2}^{\mathbf{30}}\right)_{\boldsymbol{\rho}} = \left[\left(\mathbf{i}_1^{\bar{\mathbf{X}}_i}\right)_{\boldsymbol{\rho}} + \left(\mathbf{i}_2^{\bar{\mathbf{X}}_i}\right)_{\boldsymbol{\rho}}\otimes_2\mathbf{b}_i\right]\otimes_2\mathbf{q}_f^i = \left(\mathbf{m}_{rr2}^{\mathbf{30}}\right)_{\mathbf{q}_f^i\boldsymbol{\rho}}\otimes_2\mathbf{q}_f^i \tag{129b}$$

$$\left(\mathbf{M}_{rr2}^{\mathbf{33}}\right)_{\boldsymbol{\rho}} = \left(\mathbf{i}_2^{\bar{\mathbf{X}}_i}\right)_{\boldsymbol{\rho}}\otimes_3\mathbf{q}_f^i = \left(\mathbf{M}_{rr2}^{\mathbf{33}}\right)_{\mathbf{q}_f^i\boldsymbol{\rho}}\otimes_3\mathbf{q}_f^i \tag{129c}$$

$$\left(m^{\mathbf{00}}_{rr2}\right)_{\boldsymbol{\rho}} = \left(m^{\mathbf{00}}_{rr2}\right)_{\mathbf{q}^i_f} \otimes_2 \mathbf{q}^i_f = \mathbf{b}^{\mathrm{T}}_i \left(\mathbf{m}^{\mathbf{30}}_{rr2}\right)_{\boldsymbol{\rho}} \tag{129d}$$

$$\left(\mathbf{m}^{\mathbf{03}}_{rr2}\right)_{\boldsymbol{\rho}} = \left(\mathbf{m}^{\mathbf{03}}_{rr2}\right)_{\mathbf{q}^i_f\boldsymbol{\rho}} \otimes_2 \mathbf{q}^i_f = \mathbf{b}^{\mathrm{T}}_i \left(\mathbf{M}^{\mathbf{33}}_{rr2}\right)_{\boldsymbol{\rho}} \tag{129e}$$

where extra dimensions of size 1 have been assumed for $\left(m^{\mathbf{00}}_{rr2}\right)_{\boldsymbol{\rho}} \in \mathbb{R}^{1\times1\times p}$, $\left(\mathbf{m}^{\mathbf{03}}_{rr2}\right)_{\boldsymbol{\rho}} \in \mathbb{R}^{1\times3\times p}$ and $\left(\mathbf{m}^{\mathbf{30}}_{rr2}\right)_{\boldsymbol{\rho}} \in \mathbb{R}^{3\times1\times p}$ in order to be assembled in (129). Multidimensional matrix $\left(\mathbf{i}^{\bar{\mathbf{X}}_i}_2\right)_{\boldsymbol{\rho}} \in \mathbb{R}^{3\times3\times n^i_f\times p}$ is constant during each whole simulation, or as long as the parameters are not changed:

$$\left(\mathbf{i}^{\bar{\mathbf{X}}_i}_2\right)_{\boldsymbol{\rho}} = \left(\bar{\mathbf{X}}^{-1}_i\right)_{\boldsymbol{\rho}} \otimes_2 \mathbf{i}^i_2 \otimes_2 \bar{\mathbf{X}}^{-\mathrm{T}}_i + \bar{\mathbf{X}}^{-1}_i \left(\mathbf{i}^i_2\right)_{\boldsymbol{\rho}} \otimes_2 \bar{\mathbf{X}}^{-\mathrm{T}}_i + \left(\bar{\mathbf{X}}^{-1}_i \mathbf{i}^i_2 \otimes_2 \left(\bar{\mathbf{X}}^{-1}_i\right)^{\mathrm{T}_3}_{\boldsymbol{\rho}}\right)^{\mathrm{T}_{1,2}} \tag{130}$$

$$\left(\mathbf{i}^i_2\right)_{\boldsymbol{\rho}} = \left(\mathbf{i}^i_4\right)_{\boldsymbol{\rho}} - \left(\left[\left(\mathbf{i}^i_1\right)_{\boldsymbol{\rho}} \otimes \bar{\mathbf{r}}_0\right]^{\mathrm{T}_{1,4}}\right)^{\mathrm{T}_{1,3}} - \left[\mathbf{i}^i_1 \otimes \left(\bar{\mathbf{r}}_0\right)_{\boldsymbol{\rho}}\right]^{\mathrm{T}_{1,4}} \tag{131}$$

$$\left(\mathbf{i}^i_4\right)_{\boldsymbol{\rho}} = \int_i \left[\left(\bar{\boldsymbol{\varphi}}_{\boldsymbol{\rho}} \otimes \bar{\mathbf{r}}\right)^{\mathrm{T}_{1,4}}\right]^{\mathrm{T}_{1,3}} \mathrm{d}m + \int_{\partial i} \left(\bar{\boldsymbol{\varphi}} \otimes \bar{\mathbf{r}}\right)^{\mathrm{T}_1} \mathrm{d}m \tag{132}$$

with, $\left(\mathbf{i}^i_2\right)_{\boldsymbol{\rho}}, \left(\mathbf{i}^i_4\right)_{\boldsymbol{\rho}} \in \mathbb{R}^{3\times3\times n^i_f\times p}$ constant, fourth order multidimensional matrices.

Observe that the terms for $\left(\mathbf{M}_{rr2}\right)_{\mathbf{q}^i\boldsymbol{\rho}}$ and $\left(\mathbf{M}_{rf1}\right)_{\mathbf{q}^i\boldsymbol{\rho}}$ are implicitly defined in (129).

Terms $\left(\mathbf{M}_{rr4}\right)_{\boldsymbol{\rho}}$ and $\left(\mathbf{M}_{rf2}\right)_{\boldsymbol{\rho}}$ are built with the following derivatives:

$$\left(\mathbf{T}_{rr4}\right)_{\boldsymbol{\rho}} = \begin{bmatrix} \mathbf{T}^{\mathbf{00}}_{rr4} \,\big|_2\, \mathbf{T}^{\mathbf{30}}_{rr4} \\ \mathbf{T}^{\mathbf{03}}_{rr4} \,\big|_2\, \mathbf{i}^{\bar{\mathbf{X}}_i}_3 \end{bmatrix}_{\boldsymbol{\rho}} = \begin{bmatrix} \left(\mathbf{T}^{\mathbf{00}}_{rr4}\right)_{\boldsymbol{\rho}} \,\big|_2\, \left(\mathbf{T}^{\mathbf{30}}_{rr4}\right)_{\boldsymbol{\rho}} \\ \left(\mathbf{T}^{\mathbf{03}}_{rr4}\right)_{\boldsymbol{\rho}} \,\big|_2\, \left(\mathbf{i}^{\bar{\mathbf{X}}_i}_3\right)_{\boldsymbol{\rho}} \end{bmatrix} \tag{133}$$

$$\left(\mathbf{T}^{\mathbf{00}}_{rr4}\right)_{\boldsymbol{\rho}} = \mathbf{b}^{\mathrm{T}}_i \left[\left(\mathbf{i}^{\bar{\mathbf{X}}_i}_3\right)_{\boldsymbol{\rho}} \otimes_2 \mathbf{b}_i\right] \tag{134}$$

$$\left(\mathbf{T}^{\mathbf{03}}_{rr4}\right)_{\boldsymbol{\rho}} = \left(\mathbf{i}^{\bar{\mathbf{X}}_i}_3\right)_{\boldsymbol{\rho}} \otimes_2 \mathbf{b}_i \tag{135}$$

$$\left(\mathbf{T}^{\mathbf{30}}_{rr4}\right)_{\boldsymbol{\rho}} = \mathbf{b}^{\mathrm{T}}_i \left(\mathbf{i}^{\bar{\mathbf{X}}_i}_3\right)_{\boldsymbol{\rho}} \tag{136}$$

with,

$$\begin{aligned} \left(\mathbf{i}^{\bar{\mathbf{X}}_i}_3\right)_{\boldsymbol{\rho}} &= \left(\bar{\mathbf{X}}^{-1}_i \left(\mathbf{i}^i_3\right)^{\mathrm{T}_{2,4}} \otimes_2 \bar{\mathbf{X}}^{-\mathrm{T}}_i\right)_{\boldsymbol{\rho}} = \left(\bar{\mathbf{X}}^{-1}_i\right)_{\boldsymbol{\rho}} \otimes_2 \left(\mathbf{i}^i_3\right)^{\mathrm{T}_{2,4}} \otimes_2 \bar{\mathbf{X}}^{-\mathrm{T}}_i + \\ &+ \bar{\mathbf{X}}^{-1}_i \left(\mathbf{i}^i_3\right)^{\mathrm{T}_{2,4,5}}_{\boldsymbol{\rho}} \otimes_2 \bar{\mathbf{X}}^{-\mathrm{T}}_i + \left(\left(\bar{\mathbf{X}}^{-1}_i\right)_{\boldsymbol{\rho}} \otimes_2 \left(\left(\mathbf{i}^i_3\right)^{\mathrm{T}_{2,4}}\right)^{\mathrm{T}_{3,4}} \otimes_2 \bar{\mathbf{X}}^{-\mathrm{T}}_i\right)^{\mathrm{T}_{3,4,5}} \end{aligned} \tag{137}$$

$$\left(\mathbf{i}^i_3\right)_{\boldsymbol{\rho}} = \int_i \left[\left(\bar{\boldsymbol{\varphi}}^{\mathrm{T}_3}_{\boldsymbol{\rho}} \otimes \bar{\boldsymbol{\varphi}}^{\mathrm{T}}\right)^{\mathrm{T}_{1,2,4}} + \bar{\boldsymbol{\varphi}}^{\mathrm{T}} \otimes \bar{\boldsymbol{\varphi}}_{\boldsymbol{\rho}}\right] \mathrm{d}m + \int_{\partial i} \bar{\boldsymbol{\varphi}}^{\mathrm{T}} \otimes \bar{\boldsymbol{\varphi}} \mathrm{d}m \tag{138}$$

and $\left(\mathbf{i}^i_3\right)_{\boldsymbol{\rho}} \in \mathbb{R}^{n^i_f\times3\times3\times n^i_f\times p}$, a constant fifth order multidimensional matrix.

The last term,

$$(\mathbf{M}_{ff})_{\boldsymbol{\rho}} = \int_i \left(\bar{\boldsymbol{\varphi}}_{\boldsymbol{\rho}}^{\mathrm{T}_3} \otimes_2 \bar{\boldsymbol{\varphi}} + \bar{\boldsymbol{\varphi}}^{\mathrm{T}} \bar{\boldsymbol{\varphi}}_{\boldsymbol{\rho}}\right) \mathrm{d}m = \\ = \begin{bmatrix} \left(m_{ff}^{11}\right)_{\boldsymbol{\rho}} & \Big|_2 & \left(m_{ff}^{12}\right)_{\boldsymbol{\rho}} & \Big|_2 \cdots \Big|_2 & \left(m_{ff}^{1n_f^i}\right)_{\boldsymbol{\rho}} \\ \left(m_{ff}^{21}\right)_{\boldsymbol{\rho}} & \Big|_2 & \left(m_{ff}^{22}\right)_{\boldsymbol{\rho}} & \Big|_2 \cdots \Big|_2 & \left(m_{ff}^{2n_f^i}\right)_{\boldsymbol{\rho}} \\ \vdots & \Big|_2 & \vdots & \Big|_2 \vdots \Big|_2 & \vdots \\ \left(m_{ff}^{n_f^i 1}\right)_{\boldsymbol{\rho}} & \Big|_2 & \left(m_{ff}^{n_f^i 2}\right)_{\boldsymbol{\rho}} & \Big|_2 \cdots \Big|_2 & \left(m_{ff}^{n_f^i n_f^i}\right)_{\boldsymbol{\rho}} \end{bmatrix} \tag{139}$$

$$\left(m_{ff}^{ij}\right)_{\boldsymbol{\rho}} = \left[\left(m_{ff}^{ij}\right)_{\rho_1} \Big|_3 \ldots \Big|_3 \left(m_{ff}^{ij}\right)_{\rho_p}\right] \in \mathbb{R}^{1\times 1\times p} \tag{140}$$

$$\left(m_{ff}^{jk}\right)_{\rho_l} = \mathrm{tr}\left(\left(\mathbf{i}_3\right)_{\boldsymbol{\rho}}(j,:,:,k,l)\right) \tag{141}$$

5 Numerical examples

The dynamic and sensitivity methods presented above have been implemented in the general purpose multibody library MBSLIM [11], capable of kinematic, dynamic and sensitivity analyses and optimization of rigid multibody systems with global and topological methods. Time integration in both dynamic and sensitivity systems of equations is carried out by means of the implicit trapezoidal rule.

Deformation modes have been calculated by means of the in-house finite element library FORDINA3D which performs dynamic and static analysis of finite element models using multiple types of elements. It also supports the sensitivity analysis of the former problems, delivering as result the sensitivities of the deformation modes with respect to geometric parameters. The library has been written in FORTRAN and integrated in the multibody library MBSLIM.

All the terms required in the commented flexible dynamic and sensitivity formulations have been programmed in FORTRAN taking advantage of the latest features of the language. The implementation has been tested in two numerical experiments: a benchmark fivebar problem with one of its bars considered as flexible and a more complex vehicle with a flexible chassis.

5.1 Five-bar mechanism

The five-bar mechanism has been used as benchmark experiment in multiple dynamic formulations [12] and sensitivity formulations [20, 21, 13, 19] and it is thoroughly documented in [27]. This rigid multibody model has been altered to include the flexibility of one of its bars while maintaining the mass and length of the original rigid bar. The modified flexible benchmark problem has been described and uploaded in [28] where the details of the model can be consulted.

The mechanism consists of 4 rigid bars (one of which is fixed) and one flexible bar between points 1 and 2 of Fig. 2. The flexible bar is made of steel ($E = 2.0694\times10^{11}$ Pa,

$\nu = 0.288$ and $\rho = 7.829 \times 10^3\,\mathrm{kg/m^3}$) with a length of $L_{12} = 0.5\sqrt{13}\,\mathrm{m}$ and a rectangular cross-section of $7.29 \times 10^{-3}\,\mathrm{m} \times 14.58 \times 10^{-3}\,\mathrm{m}$. The orientation of the flexible bar is such that its largest cross-sectional dimension coincides with the axis of the revolute joints.

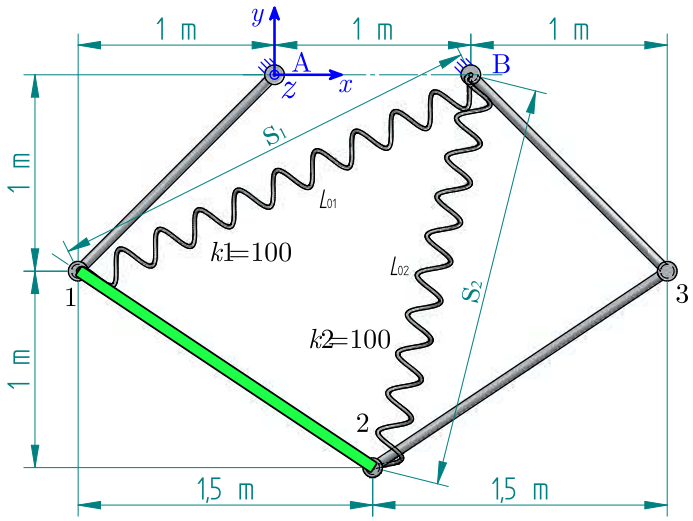


Fig. 2: Five-bar mechanism

The mechanism is subjected to the action of gravity and two spring forces. A 5-second maneuver is simulated with a 2×10^{-3} second time step and implicit trapezoidal rule as numerical integrator. The ALI3 penalty coefficient is set to 10^{10}, while non-iterative mass orthogonal projections are used with $\varsigma = 10^{-5}$.

The flexibility is parameterized by means of 14 modes of deformation coming from a modal analysis of the bar with its tip faces behaving as rigid bodies with $Y-$translation and $X-$ and $Z-$rotations impeded. As long as the revolute joints at points 1 and 2 are modeled as ideal joints, 1 point and 1 vector are shared between bodies, which implies that the deformation of the bar is constrained. That is why boundary constraints on the tip faces during the modal analysis have been considered. The model generated with this deformation modes has redundant constraints, but the ALI3-P dynamic and sensitivity equations can deal with them.

Fig. 3 compares the acceleration of the X and Y coordinate of point 2 between the flexible and rigid body cases. The accelerations of both models are almost identical except for a non-negligible ripple in the flexible case stemming from the oscillations of the flexible bar due to deformation.

The sensitivity analysis of the dynamics of the mechanism is studied considering the set of parameters of the flexible benchmark problem [27], which are the natural lengths of the springs and the mass, the X coordinate of the center of mass, the lengths

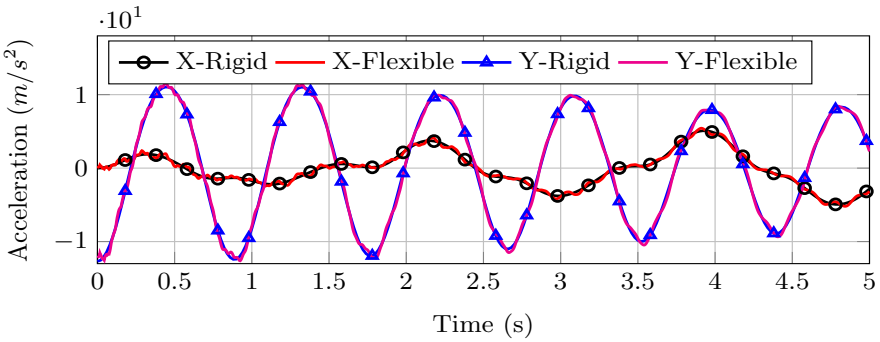


Fig. 3: Components X and Y of the acceleration of point 2.

of the rigid bar A1 and the length of the flexible bar 12[6]:

$$\boldsymbol{\rho} = \begin{bmatrix} L_{s1} & L_{s2} & m_{A1} & \bar{x}^G_{A1} & L_{A1} & L_{12} \end{bmatrix} \tag{142}$$

The sensitivity analysis is used to compute the gradient of the array of objective functions $\boldsymbol{\psi}^{\mathrm{T}} = \begin{bmatrix} \psi^1 & \psi^2 & \psi^3 \end{bmatrix}$, with

$$\psi^1 = \int_{t_0}^{t_F} (\mathbf{r}_2 - \mathbf{r}_{20})^{\mathrm{T}} (\mathbf{r}_2 - \mathbf{r}_{20}) \, \mathrm{d}t, \quad \psi^2 = \int_{t_0}^{t_F} \dot{\mathbf{r}}_2^{\mathrm{T}} \dot{\mathbf{r}}_2 \mathrm{d}t, \quad \psi^3 = \int_{t_0}^{t_F} \ddot{\mathbf{r}}_2^{\mathrm{T}} \ddot{\mathbf{r}}_2 \mathrm{d}t. \tag{143}$$

being $\mathbf{r}_{20} = \begin{bmatrix} 0.5 & -2.0 & 0 \end{bmatrix}$, therefore, applying equation (74),

$$\boldsymbol{\psi}' = \begin{bmatrix} \psi^{1\prime} \\ \psi^{2\prime} \\ \psi^{3\prime} \end{bmatrix} = \int_{t_0}^{t_F} \begin{bmatrix} (\mathbf{r}_2 - \mathbf{r}_{20})^{\mathrm{T}} \mathbf{r}_2' \\ \dot{\mathbf{r}}_2^{\mathrm{T}} \dot{\mathbf{r}}_2' \\ \ddot{\mathbf{r}}_2^{\mathrm{T}} \ddot{\mathbf{r}}_2' \end{bmatrix} \mathrm{d}t \tag{144}$$

Table 1 presents the gradients of the objective functions (143) obtained using the sensitivity analysis methods presented in this paper. Gradient results are compared with numerical differentiation (by means of finite real differences), giving evidence of the validity of the analytical calculation, and against the rigid body case, which differs from the flexible solution. The difference between sensitivities for the rigid and flexible multibody examples is displayed in Fig. 4.

Additionally, Fig. 5 shows the evolution of each component of the gradient of the objective function ψ_3 for the rigid an flexible five-bar mechanisms. Analogous figures can be obtained for the objective functions ψ_1 and ψ_2.

The dynamic and sensitivity analysis calculation requires 2.54 seconds to be executed (discarding preprocess time). This means that both the dynamics of the flexible 5-bar mechanism and its sensitivities with respect to 6 design parameters can be simulated in 1.97 times Real Time with the approach proposed.

[6]Details on how to compute analytically the partial derivatives with respect to a parameter affecting the geometry of a flexible body are out of the scope of this work.

	Rigid	Flexible	
		Analytical	Numerical
$(\psi^1)'_{L_{s1}}$	-4.2288	-4.2332	-4.2428
$(\psi^1)'_{L_{s2}}$	3.2116	3.2023	3.2057
$(\psi^1)'_{m_{A1}}$	0.31864	0.31883	0.31852
$(\psi^1)'_{x^G_{A1}}$	0.44233	0.44256	0.44145
$(\psi^1)'_{L_{A1}}$	3.3599	3.3737	3.3372
$(\psi^1)'_{L_{12}}$	1.1853	1.1874	1.1895
$(\psi^2)'_{L_{s1}}$	-15.452	-15.505	-15.463
$(\psi^2)'_{L_{s2}}$	50.309	50.201	50.263
$(\psi^2)'_{m_{A1}}$	0.97023	0.96939	0.96218
$(\psi^2)'_{x^G_{A1}}$	0.74589	0.74406	0.73113
$(\psi^2)'_{L_{A1}}$	-27.360	-27.188	-27.199
$(\psi^2)'_{L_{12}}$	-16.487	-16.369	-16.372
$(\psi^3)'_{L_{s1}}$	221.66	223.30	223.57
$(\psi^3)'_{L_{s2}}$	2436.6	2409.7	2412.5
$(\psi^3)'_{m_{A1}}$	-32.496	-32.912	-33.186
$(\psi^3)'_{x^G_{A1}}$	-85.663	-86.502	-87.219
$(\psi^3)'_{L_{A1}}$	-2546.7	-2525.2	-2523.6
$(\psi^3)'_{L_{12}}$	-704.08	-690.29	-690.78

Table 1: Objective-function-gradient values for the five-bar mechanism.

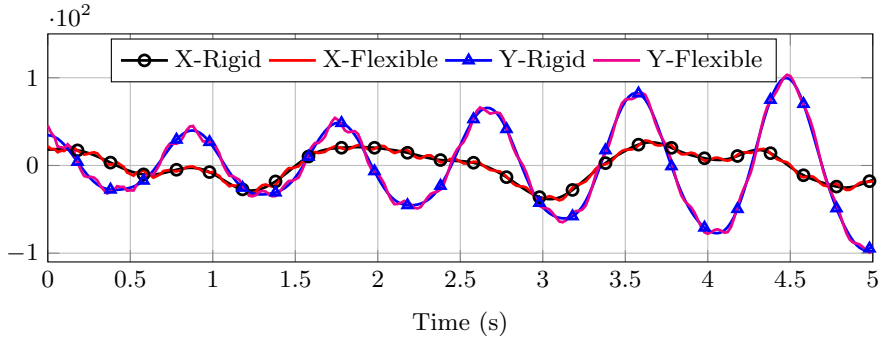


Fig. 4: Sensitivity of the X and Y components of the acceleration of point 2 with respect to L_{12}.

5.2 Buggy vehicle

A more complex sensitivity benchmark problem is considered to check both the validity and the generality of the sensitivity formulation proposed. The multibody model studied is the four-wheeled buggy vehicle displayed in Fig. 6, which consists of 18 movable bodies articulated by means of diverse kinematic joints. The system is subjected to the action of different forces, such as gravity, spring-damper forces coming from the suspension systems or normal-frictional tire forces. The reader is referred to [27] for a thorough description of the rigid multibody model.

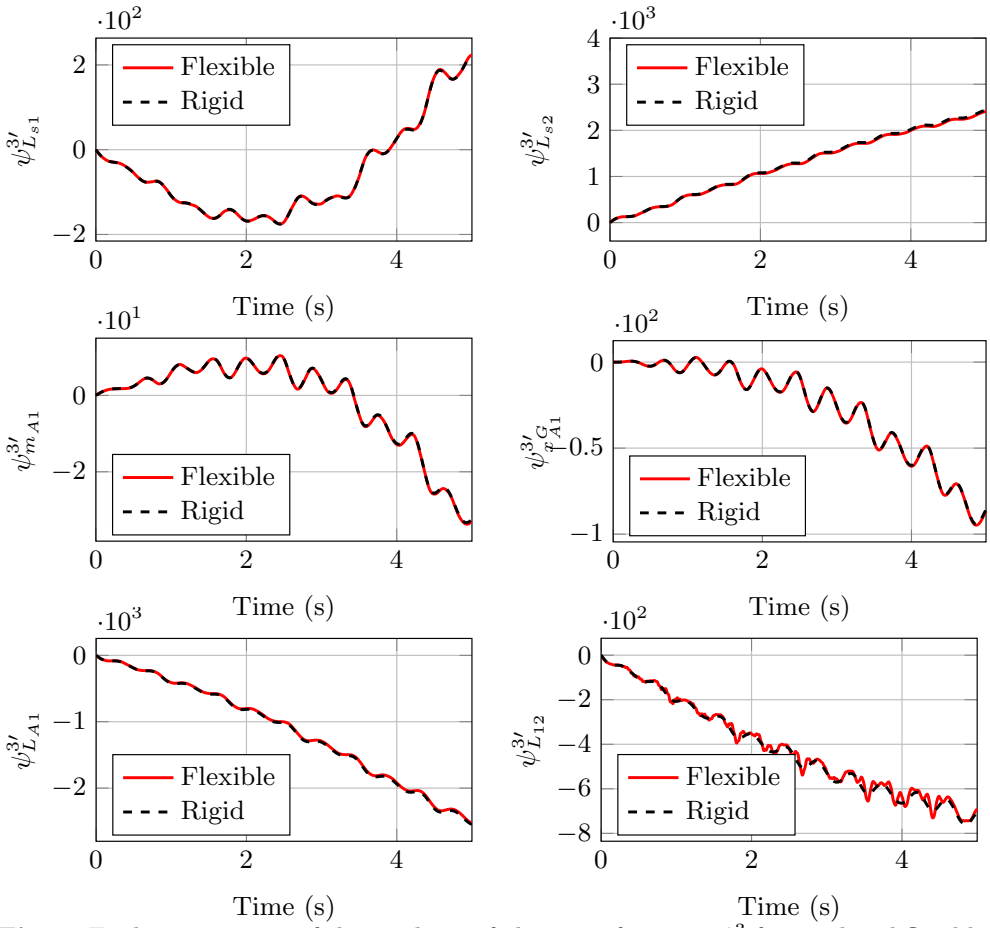


Fig. 5: Evolution in time of the gradient of objective function ψ^3 for rigid and flexible multibody models

The original model has been updated to include the flexibility of the chassis, but preserving the original mass distribution of the former rigid-body model. The flexibility of the chassis is defined by 10 elastic coordinates which represent the modal amplitudes of the set of deformation modes shown Fig. 7, obtained through modal analysis[7]. Rigid body vectors shared between chassis and other bodies in the original rigid body model have been substituted by flexible vectors defined by means of two flexible points. The extended flexible model involves 304 coordinates (10 of which are flexible modal amplitudes) and is subjected to 292 constraints, 12 of them redundant.

The maneuver studied consists in a 1cm-step descent, according to [27]. The vehicle moves forward with the wheels aligned by means of a rheonomous driving constraint, with all the kinetic energy coming from its initial velocity.

[7]Information regarding the geometry and material properties of the chassis can be made available upon request.

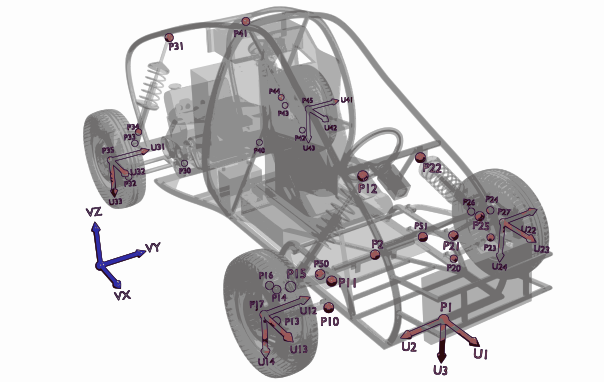
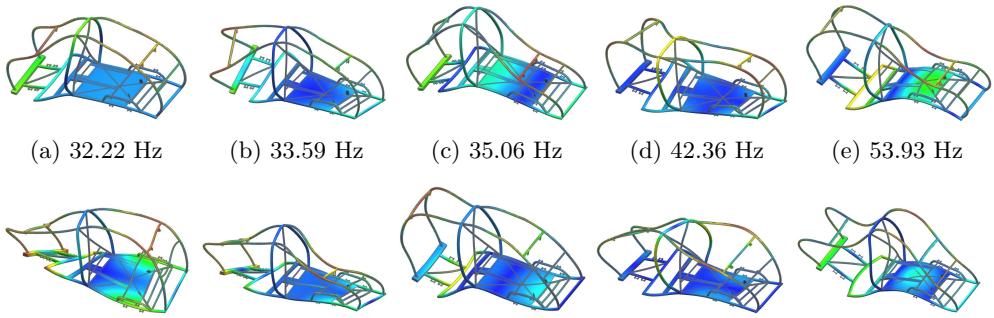


Fig. 6: Buggy vehicle



(a) 32.22 Hz (b) 33.59 Hz (c) 35.06 Hz (d) 42.36 Hz (e) 53.93 Hz

(f) 58.77 Hz (g) 58.77 Hz (h) 58.77 Hz (i) 58.77 Hz (j) 58.77 Hz

Fig. 7: Deformation modes of the flexible chassis (in this case, all of them are dynamic)

The numerical simulation is executed with a time step of 5×10^{-4} seconds and the implicit trapezoidal rule as numerical integrator. The ALI3 penalty coefficient is set to 4×10^{10}, while non-iterative mass orthogonal projections are used with $\varsigma = 2.5 \times 10^{-8}$.

The evolution of the acceleration of point 1 in the Z direction is presented in Fig. 8 for the rigid and the flexible body cases. A non-negligible difference can be observed between the results of the two models, with the flexible model experimenting higher accelerations at the initial instant of time (the initial position does not coincide with the static equilibrium position) and lower accelerations at the step descent.

The objective function considered for the sensitivity analysis consists in a measure of the pilot comfort:

$$\psi = \int_{t_0}^{t_F} \ddot{r}_{1z}^2 \mathrm{d}t \tag{145}$$

with $\ddot{r}_{1z}$ identifying the Z-component of the acceleration of a point located in the front of the chassis.

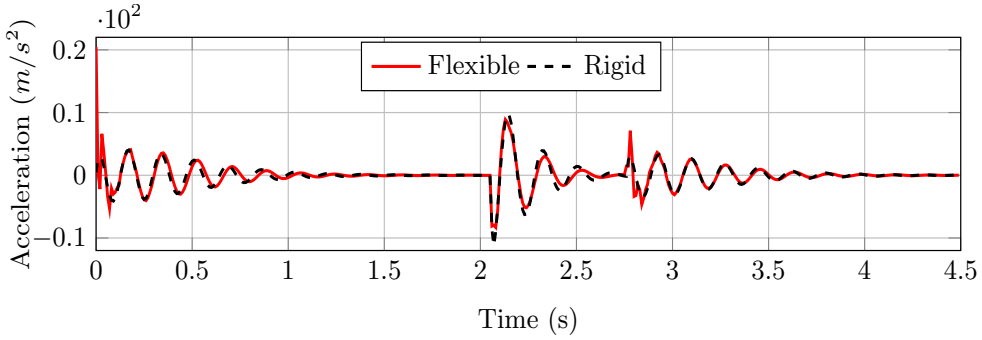


Fig. 8: Evolution of Z-component of the acceleration of point 1.

The stiffness (k) and damping coefficients (c) of the front and rear suspensions represent the set of sensitivity parameters. In the rigid body benchmark, the chassis mass was also a parameter, but in the flexible problem it cannot be considered since the mass is a sub-product of the dynamic pre-process, not an independent quantity.

$$\boldsymbol{\rho} = \begin{bmatrix} k_f & c_f & k_r & c_r \end{bmatrix} \tag{146}$$

Therefore, the gradient of (145) can be obtained, according to (74),

$$\psi' = \frac{\mathrm{d}\psi}{\mathrm{d}\boldsymbol{\rho}} = \int_{t_0}^{t_F} \mathbf{g}_{\ddot{\mathbf{q}}} \ddot{\mathbf{q}}' \, \mathrm{dt} = \int_{t_0}^{t_F} 2\ddot{r}_{1z} \ddot{\mathbf{r}}'_{1z} \mathrm{d}t \tag{147}$$

The objective function evolution is notably affected by the flexibility of the chassis, according to Fig. 9. The difference grows bigger in sensitivities. Fig. 10 evidences the significant effect of the consideration of flexibility in the gradient components of the objective function (145). In this numerical problem, the analytical gradient values have been validated against numerical differentiation through real finite differences.

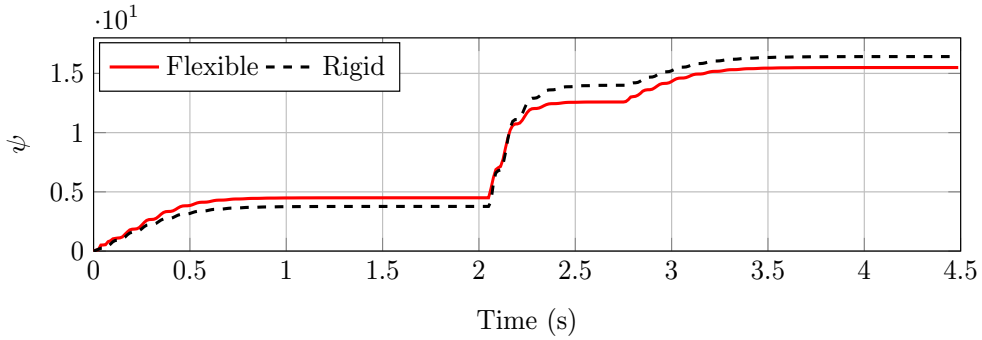


Fig. 9: Evolution of the objective function of the step-descent maneuver.

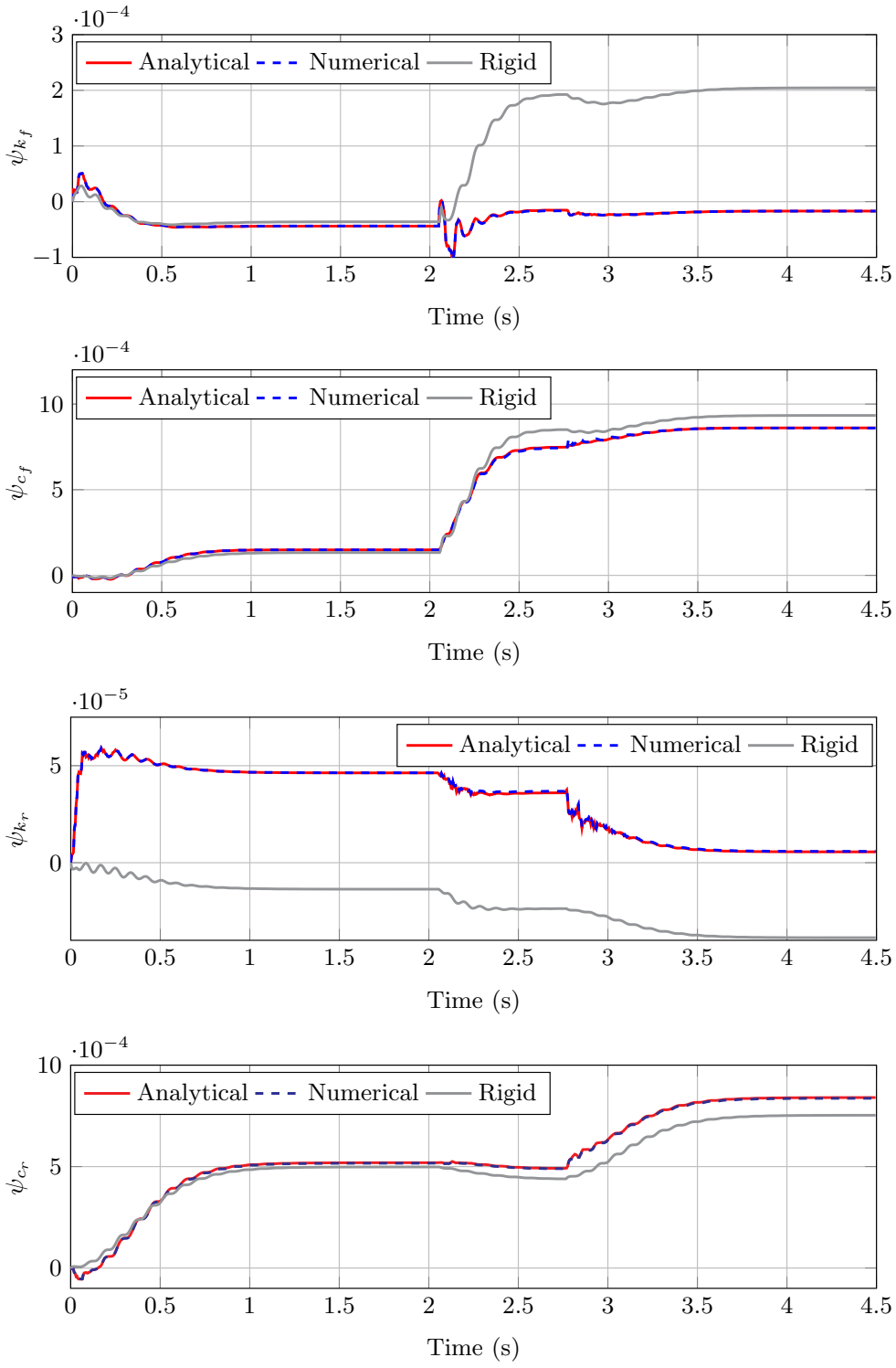


Fig. 10: Evolution in time of the gradient of ψ for rigid and flexible multibody models

The computation of analytical sensitivities requires approximately a 58.5% of the time devoted to the dynamics simulation[8], while numerical sensitivities require a 400%. The higher the number of sensitivity parameters, the greater the differences.

6 Conclusions

A general formulation for the sensitivity analysis of the dynamics of flexible multibody systems based on analytical expressions is thoroughly derived.

The kinematics of flexible bodies is based on a novel description for natural coordinates along with the Floating Frame of Reference (FFR) description of deformation. The advantages of using FFR are twofold: the equations and the resulting code are modular and the sensitivities with rigid bodies are an extension of the rigid body ones; the approach is very efficient because of the low number of flexible coordinates compared to nonlinear finite element formulations in nodal coordinates and this is mandatory because the final goal of the sensitivities is optimization.

The approach adopted for FFR uses a Bucken's frame, thus no attachment conditions are *a priori* impossed, between the body and the frame, which is truly floating and more versatile than the classical tangent frames usually adopted with natural coordinates. If a tangent frame is desired, it is still possible to imposse it from this approach, by a proper selection of deformation modes and constraints.

The motivation of the work was the extension of the rigid body MBSLIM formulations to accomodate flexible bodies. This imposed restrictions of generality on the approach, compared to previous works presented in the bibliography.

The mass matrix of a flexible body is divided on rigid, flexible and coupling terms and the shape integrals are built on the basis of the classical integrals for rigid (mass, center of mass and inertia tensor) and only three integrals for the flexible and coupling terms (a matrix, a three dimensional matrix and a four dimensional one). The elemental mass matrix is built with those pieces, resulting in constant, linear and quadratic terms on the states. Therefore, the derivatives of the mass matrix with respect to the states, are built with constant and at most linear terms which renders the method very efficient. Moreover, the method does not need the introduction of any extra states or constraints in addition to the flexible modal coordinates, which keeps the size of the problem as small as possible.

For the sake of simplicity, the work was focused on the ALI3-P formulation of the equations of motion and direct sensitvities but the expressions provided allow the extension for other formulations available in MBSLIM and for adjoint sensitivities as well. For this reason, the theory and implementation strongly relies on the multidimensional matrix algebra, with the aim of minimizing the amount of code, because the same terms appear in different formulations of the equations of motion but combined differently. The same happens if direct and adjoint sensitivities are compared, the same individual terms are needed for both of them and the tensor algebra approach allows to make use of a minimal number of terms and code.

[8] The time devoted to the pre-process and model generation before the simulation has not been considered for the comparison of computational times.

Acknowledgments

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A Multidimensional matrix algebra

A high-order matrix is defined as a matrix of more than 2 dimensions. It can be also expressed as a concatenation of matrices. As an example, a 3-order matrix can be defined in terms of regular matrices as:

$$\left\{\mathbf{T} \in \mathbb{R}^{m\times n\times o}, \mathbf{O}_i \in \mathbb{R}^{m\times n}, \mathbf{T} = \left[\mathbf{O}_1\middle|_3 ... \middle|_3 \mathbf{O}_o\right]\right\} \tag{148}$$

or

$$\left\{\mathbf{T} \in \mathbb{R}^{m\times n\times o}, \mathbf{N}_i \in \mathbb{R}^{m\times o}, \mathbf{T} = \left[\mathbf{N}_1\middle|_2 ... \middle|_2 \mathbf{N}_n\right]\right\} \tag{149}$$

or

$$\left\{\mathbf{T} \in \mathbb{R}^{m\times n\times o}, \mathbf{M}_i \in \mathbb{R}^{n\times o}, \mathbf{T} = \begin{bmatrix}\mathbf{M}_1\\ ...\\ \mathbf{M}_m\end{bmatrix}\right\} \tag{150}$$

In addition to the inner and outer products, the following products can be defined with high-order matrices:

1. Mode 2 product:

$$\left\{\mathbf{T} \in \mathbb{R}^{m\times n\times o}, \mathbf{M} \in \mathbb{R}^{n\times p}, \mathbf{T} \otimes_2 \mathbf{M} = \left[\mathbf{T}_{(:,:,1)}\mathbf{M}\middle|_3 ... \middle|_3 \mathbf{T}_{(:,:,o)}\mathbf{M}\right]\right\} \tag{151}$$

2. Mode 3 product:

$$\left\{\mathbf{T} \in \mathbb{R}^{m\times n\times o}, \mathbf{N} \in \mathbb{R}^{o\times p}, \mathbf{T} \otimes_3 \mathbf{M} = \left[\mathbf{T}_{(:,1,:)}\mathbf{M}\middle|_2 ... \middle|_2 \mathbf{T}_{(:,n,:)}\mathbf{M}\right]\right\} \tag{152}$$

3. Mode 4 product:

$$\left\{\mathbf{R} \in \mathbb{R}^{m\times n\times o\times p}, \mathbf{O} \in \mathbb{R}^{p\times q}, \mathbf{R} \otimes_4 \mathbf{O} = \left[\mathbf{R}_{(:,:,1,:)} \otimes_3 \mathbf{O}\middle|_3 ... \middle|_3 \mathbf{R}_{(:,:,o,:)} \otimes_3 \mathbf{O}\right]\right\} \tag{153}$$

Higher order products with higher order matrices can be defined in terms of the listed products.

Mode-x products have the following properties:

1. Commutativity if the mode of the product is different:

$$\mathbf{T} \otimes_2 \mathbf{M} \otimes_3 \mathbf{N} = \mathbf{T} \otimes_3 \mathbf{N} \otimes_2 \mathbf{M} \tag{154}$$

2. Associativity with equal mode products:

$$\mathbf{T} \otimes_2 \mathbf{M} \otimes_2 \mathbf{N} = (\mathbf{T} \otimes_2 \mathbf{M}) \otimes_2 \mathbf{N} = \mathbf{T} \otimes_2 (\mathbf{MN}) \tag{155}$$

3. Neutral element:

$$\mathbf{T} \otimes_2 \mathbf{I}_n = \mathbf{T} \otimes_3 \mathbf{I}_o = \mathbf{T} \tag{156}$$

As long as high order matrices have more than 3 dimensions, the transpose operation requires additional information to indicate which are the dimensions to transpose. Let is consider a 3-order matrix $\mathbf{T}$. The transpose of the 1^{st} and 2^{nd} dimensions is indicated in this work as $\mathbf{T}^{\mathrm{T}_3}$, where the index of the transpose marks the dimension that remains unaltered. Therefore, the transposition of the 1^{st} and 3^{rd} dimensions is denoted as $\mathbf{T}^{\mathrm{T}_2}$, while $\mathbf{T}^{\mathrm{T}_1}$ identifies the transpose of the 2^{nd} and 3^{rd} dimensions.

B Mass matrix shape integrals

The expressions of the shape integrals for the elemental mass matrix of a flexible body in natural coordinates are provided in this section. They are written as dense matrices but sparsity should be exploited. The final expressions are linear or bilinear expressions of $\mathbf{q}_r^i$, $\mathbf{q}_f^i$, then, most of the calculations can be done before starting the simulation and stored.

B.1 Block $\mathbf{M}_{rr}^i$

The first integral $\mathbf{M}_{rr1}$ of the first block $\mathbf{M}_{rr}^i$ needs for the following integrals:

$$\mathbf{M}_{rr1}^{4\times4} = \int_i \bar{\mathbf{c}}\bar{\mathbf{c}}^{\mathrm{T}} \mathrm{d}m = \int_i \begin{bmatrix} \bar{c}_0^2 & \bar{c}_0\bar{\mathbf{c}}^{3\mathrm{T}} \\ \bar{\mathbf{c}}^3\bar{c}_0 & \bar{\mathbf{c}}^3\bar{\mathbf{c}}^{3\mathrm{T}} \end{bmatrix} \mathrm{d}m = \int_i \begin{bmatrix} \bar{c}_0^2 & \bar{c}_0\bar{c}_1 & \bar{c}_0\bar{c}_2 & \bar{c}_0\bar{c}_3 \\ \bar{c}_1\bar{c}_0 & \bar{c}_1^2 & \bar{c}_1\bar{c}_2 & \bar{c}_1\bar{c}_3 \\ \bar{c}_2\bar{c}_0 & \bar{c}_2\bar{c}_1 & \bar{c}_2^2 & \bar{c}_2\bar{c}_3 \\ \bar{c}_3\bar{c}_0 & \bar{c}_3\bar{c}_1 & \bar{c}_3\bar{c}_2 & \bar{c}_3^2 \end{bmatrix} \mathrm{d}m \tag{157}$$

$$\int_i \bar{\mathbf{c}}^3\bar{\mathbf{c}}^{3\mathrm{T}} \mathrm{d}m = \bar{\mathbf{X}}_i^{-1} \left(\int_i (\bar{\mathbf{r}} - \bar{\mathbf{r}}_0) (\bar{\mathbf{r}} - \bar{\mathbf{r}}_0)^{\mathrm{T}} \, \mathrm{d}m \right) \bar{\mathbf{X}}_i^{-\mathrm{T}} = \bar{\mathbf{X}}_i^{-1} \bar{\mathbf{P}}_0^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \tag{158}$$

$$\begin{aligned} \int_i \bar{c}_0\bar{\mathbf{c}}^{3\mathrm{T}} \mathrm{d}m = \left(\int_i \left(1 + \mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}^{-1} (\bar{\mathbf{r}} - \bar{\mathbf{r}}_0)\right) (\bar{\mathbf{r}} - \bar{\mathbf{r}}_0)^{\mathrm{T}} \, \mathrm{d}m \right) \bar{\mathbf{X}}_i^{-\mathrm{T}} = \\ = \left[m_i \left(\bar{\mathbf{r}}_G^i - \bar{\mathbf{r}}_0^i\right)^{\mathrm{T}} + \mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}_i^{-1} \bar{\mathbf{P}}_0^i \right] \bar{\mathbf{X}}_i^{-\mathrm{T}} \end{aligned} \tag{159}$$

$$\begin{aligned} \int_i \bar{c}_0^2 \mathrm{d}m = \int_i \left(1 + \mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}^{-1} (\bar{\mathbf{r}} - \bar{\mathbf{r}}_0)\right) \left(1 + (\bar{\mathbf{r}} - \bar{\mathbf{r}}_0)^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{b}\right) \mathrm{d}m = \\ = m_i + 2m_i \mathbf{b}_i^{\mathrm{T}} \bar{\mathbf{X}}_i^{-1} \left(\bar{\mathbf{r}}_G^i - \bar{\mathbf{r}}_0^i\right) + \mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}_i^{-1} \bar{\mathbf{P}}_0^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \mathbf{b}_i \\ = m_i + \mathbf{b}_i^{\mathrm{T}} \bar{\mathbf{X}}_i^{-1} \left[\bar{\mathbf{P}}_0^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \mathbf{b}_i + 2m_i \left(\bar{\mathbf{r}}_G^i - \bar{\mathbf{r}}_0^i\right) \right] \end{aligned} \tag{160}$$

with $\bar{\mathbf{P}}_0^i$ defined in (43).

The second integral $\mathbf{M}_{rr2}$ of the first block $\mathbf{M}_{rr}$:

$$\begin{aligned}\mathbf{M}_{rr2} &= \int_i \bar{\mathbf{C}}^{\mathrm{T}} \mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f \mathrm{d}m = \\ &= \int_i \begin{bmatrix} \bar{c}_0 \mathbf{I}_3 \\ \bar{c}_1 \mathbf{I}_3 \\ \bar{c}_2 \mathbf{I}_3 \\ \bar{c}_3 \mathbf{I}_3 \end{bmatrix} \left[\mathbf{E} \otimes_2 \mathbf{b}^{\mathrm{T}} \big|_3 \mathbf{E} \otimes_2 \mathbf{e}_1^{\mathrm{T}} \big|_3 \mathbf{E} \otimes_2 \mathbf{e}_2^{\mathrm{T}} \big|_3 \mathbf{E} \otimes_2 \mathbf{e}_3^{\mathrm{T}} \right] \otimes_2 \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \mathrm{d}m \end{aligned} \tag{161}$$

Elaborating on each element of $\mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f$ the following two expressions are obtained:

$$\mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f = \left[\mathbf{E} \otimes_2 \mathbf{b}^{\mathrm{T}} \big|_3 \mathbf{E} \otimes_2 \mathbf{e}_1^{\mathrm{T}} \big|_3 \mathbf{E} \otimes_2 \mathbf{e}_2^{\mathrm{T}} \big|_3 \mathbf{E} \otimes_2 \mathbf{e}_3^{\mathrm{T}} \right] \otimes_2 \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \tag{162a}$$

$$\left(\mathbf{E} \otimes_2 \mathbf{b}^{\mathrm{T}} \right) \otimes_2 \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f = \left(\mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \right) \mathbf{I}_3 \tag{162b}$$

$$\left(\mathbf{E} \otimes_2 \mathbf{e}_k^{\mathrm{T}} \right) \otimes_2 \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f = \left(\mathbf{e}_k^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \right) \mathbf{I}_3;\ k = 1, 2, 3. \tag{162c}$$

In equations (162) the product $\mathbf{E} \otimes_2 c = c\mathbf{I}_3$ for any scalar $c \in \mathbb{R}$ was used. Four types of terms appear in (161),

$$\left(\bar{c}_0 \mathbf{I}_3 \right) \left(\mathbf{E} \otimes_2 \mathbf{b}^{\mathrm{T}} \right) \otimes_2 \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f = \left(\bar{c}_0 \mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \right) \mathbf{I}_3 \tag{163a}$$

$$\left(\bar{c}_j \mathbf{I}_3 \right) \left(\mathbf{E} \otimes_2 \mathbf{b}^{\mathrm{T}} \right) \otimes_2 \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f = \left(\bar{c}_j \mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \right) \mathbf{I}_3;\ j = 1, 2, 3. \tag{163b}$$

$$\left(\bar{c}_0 \mathbf{I}_3 \right) \left(\mathbf{E} \otimes_2 \mathbf{e}_k^{\mathrm{T}} \right) \otimes_2 \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f = \left(\bar{c}_0 \mathbf{e}_k^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \right) \mathbf{I}_3;\ k = 1, 2, 3. \tag{163c}$$

$$\left(\bar{c}_j \mathbf{I}_3 \right) \left(\mathbf{E} \otimes_2 \mathbf{e}_k^{\mathrm{T}} \right) \otimes_2 \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f = \left(\bar{c}_j \mathbf{e}_k^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \right) \mathbf{I}_3;\ j, k = 1, 2, 3. \tag{163d}$$

The terms in parenthesis can be further expanded using (16) and (12):

$$\bar{c}_0 \mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f = \mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \left(1 + (\bar{\mathbf{r}} - \bar{\mathbf{r}}_0)^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{b} \right) \tag{164}$$

$$\bar{c}_j \mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f = \mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \left(\bar{\mathbf{r}} - \bar{\mathbf{r}}_0 \right)^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{e}_j \tag{165}$$

$$\bar{c}_0 \mathbf{e}_k^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f = \mathbf{e}_k^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \left(1 + (\bar{\mathbf{r}} - \bar{\mathbf{r}}_0)^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{b} \right) \tag{166}$$

$$\bar{c}_j \mathbf{e}_k^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f = \mathbf{e}_k^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \left(\bar{\mathbf{r}} - \bar{\mathbf{r}}_0 \right)^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{e}_j \tag{167}$$

Then $\mathbf{M}_{rr2}$ results in the following.

$$\mathbf{M}_{rr2} = \int_i \bar{\mathbf{C}}^{\mathrm{T}} \mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f \mathrm{d}m = \begin{bmatrix} m_{rr2}^{00} \mathbf{I}_3 & m_{rr2}^{01} \mathbf{I}_3 & m_{rr2}^{02} \mathbf{I}_3 & m_{rr2}^{03} \mathbf{I}_3 \\ m_{rr2}^{10} \mathbf{I}_3 & m_{rr2}^{11} \mathbf{I}_3 & m_{rr2}^{12} \mathbf{I}_3 & m_{rr2}^{13} \mathbf{I}_3 \\ m_{rr2}^{20} \mathbf{I}_3 & m_{rr2}^{21} \mathbf{I}_3 & m_{rr2}^{22} \mathbf{I}_3 & m_{rr2}^{23} \mathbf{I}_3 \\ m_{rr2}^{30} \mathbf{I}_3 & m_{rr2}^{31} \mathbf{I}_3 & m_{rr2}^{32} \mathbf{I}_3 & m_{rr2}^{33} \mathbf{I}_3 \end{bmatrix} \tag{168a}$$

$$m_{rr2}^{00} = \int_i \bar{c}_0 \mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \mathrm{d}m = \mathbf{b}_i^{\mathrm{T}} \bar{\mathbf{X}}_i^{-1} \left(\mathbf{m}_1^i + \mathbf{m}_2^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \mathbf{b}_i \right) \tag{168b}$$

$$m_{rr2}^{j0} = \int_i \bar{c}_j \mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \mathrm{d}m = \mathbf{b}_i^{\mathrm{T}} \bar{\mathbf{X}}_i^{-1} \mathbf{m}_2^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \mathbf{e}_j \tag{168c}$$

$$m_{rr2}^{0k} = \int_i \bar{c}_0 \mathbf{e}_k^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \mathrm{d}m = \mathbf{e}_k^{\mathrm{T}} \bar{\mathbf{X}}_i^{-1} \left(\mathbf{m}_1^i + \mathbf{m}_2^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \mathbf{b} \right) \tag{168d}$$

$$m_{rr2}^{jk} = \int_i \bar{c}_j \mathbf{e}_k^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \mathrm{d}m = \mathbf{e}_k^{\mathrm{T}} \bar{\mathbf{X}}_i^{-1} \mathbf{m}_2^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \mathbf{e}_j \tag{168e}$$

$$\mathbf{m}_1^i = \int_i \bar{\mathbf{r}}_f \mathrm{d}m = \left[\int_i \bar{\boldsymbol{\varphi}} \mathrm{d}m \right] \mathbf{q}_f^i = \mathbf{i}_1^i \mathbf{q}_f^i \tag{168f}$$

$$\mathbf{m}_2^i = \int_i \bar{\mathbf{r}}_f \left(\bar{\mathbf{r}} - \bar{\mathbf{r}}_0 \right)^{\mathrm{T}} \mathrm{d}m = \left[\int_i \left(\bar{\boldsymbol{\varphi}} \otimes \left(\bar{\mathbf{r}} - \bar{\mathbf{r}}_0 \right) \right)^{\mathrm{T}_1} \mathrm{d}m \right] \otimes_3 \mathbf{q}_f^i = \mathbf{i}_2^i \otimes_3 \mathbf{q}_f^i \tag{168g}$$

The final expressions of the mass matrix $\mathbf{M}_{rr2}$ given in (44) are straightforward from (168).

Terms $\mathbf{m}_1^i \in \mathbb{R}^{3\times 1}$ and $\mathbf{m}_2^i \in \mathbb{R}^{3\times 3}$ are linear functions of the states $\mathbf{q}_f^i$ with the constant integrals $\mathbf{i}_1^i \in \mathbb{R}^{3\times n_f^i}$ and $\mathbf{i}_2^i \in \mathbb{R}^{3\times 3\times n_f^i}$.

The fourth integral $\mathbf{M}_{rr4}$ of the first block $\mathbf{M}_{rr}$ is, considering (162):

$$\mathbf{M}_{rr4} = \int_i \left(\mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f \right)^{\mathrm{T}} \left(\mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f \right) \mathrm{d}m = \begin{bmatrix} m_{rr4}^{00}\mathbf{I}_3 & m_{rr4}^{01}\mathbf{I}_3 & m_{rr4}^{02}\mathbf{I}_3 & m_{rr4}^{03}\mathbf{I}_3 \\ m_{rr4}^{10}\mathbf{I}_3 & m_{rr4}^{11}\mathbf{I}_3 & m_{rr4}^{12}\mathbf{I}_3 & m_{rr4}^{13}\mathbf{I}_3 \\ m_{rr4}^{20}\mathbf{I}_3 & m_{rr4}^{21}\mathbf{I}_3 & m_{rr4}^{22}\mathbf{I}_3 & m_{rr4}^{23}\mathbf{I}_3 \\ m_{rr4}^{30}\mathbf{I}_3 & m_{rr4}^{31}\mathbf{I}_3 & m_{rr4}^{32}\mathbf{I}_3 & m_{rr4}^{33}\mathbf{I}_3 \end{bmatrix} \tag{169a}$$

$$m_{rr4}^{00} = \int_i \left(\mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \right) \left(\bar{\mathbf{r}}_f^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{b} \right) \mathrm{d}m = \mathbf{b}_i^{\mathrm{T}} \bar{\mathbf{X}}_i^{-1} \mathbf{m}_3^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \mathbf{b}_i \tag{169b}$$

$$m_{rr4}^{j0} = \int_i \left(\mathbf{e}_j^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \right) \left(\bar{\mathbf{r}}_f^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{b} \right) \mathrm{d}m = \mathbf{e}_j^{\mathrm{T}} \bar{\mathbf{X}}_i^{-1} \mathbf{m}_3^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \mathbf{b}_i \tag{169c}$$

$$m_{rr4}^{0k} = \int_i \left(\mathbf{b}^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \right) \left(\bar{\mathbf{r}}_f^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{e}_k \right) \mathrm{d}m = \mathbf{b}_i^{\mathrm{T}} \bar{\mathbf{X}}_i^{-1} \mathbf{m}_3^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \mathbf{e}_k \tag{169d}$$

$$m_{rr4}^{jk} = \int_i \left(\mathbf{e}_j^{\mathrm{T}} \bar{\mathbf{X}}^{-1} \bar{\mathbf{r}}_f \right) \left(\bar{\mathbf{r}}_f^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{e}_k \right) \mathrm{d}m = \mathbf{e}_j^{\mathrm{T}} \bar{\mathbf{X}}_i^{-1} \mathbf{m}_3^i \bar{\mathbf{X}}_i^{-\mathrm{T}} \mathbf{e}_k \tag{169e}$$

$$\mathbf{m}_3^i = \int_i \bar{\mathbf{r}}_f \bar{\mathbf{r}}_f^{\mathrm{T}} \mathrm{d}m = \left[\mathbf{q}_f^{i\mathrm{T}} \int_i \left(\bar{\boldsymbol{\varphi}}^{\mathrm{T}} \otimes \bar{\boldsymbol{\varphi}} \right) \mathrm{d}m \right] \otimes_3 \mathbf{q}_f^i = \left[\mathbf{q}_f^{i\mathrm{T}} \mathbf{i}_3^i \right] \otimes_3 \mathbf{q}_f^i \tag{169f}$$

From equations (169), the derivation of $\mathbf{M}_{rr4}$ in section 3.3.1 is straightforward. The following identity has been used in the derivations:

$$\bar{\mathbf{X}}_i^{-1} \left[\left(\mathbf{q}_f^{i\mathrm{T}} \mathbf{i}_3^i \right) \otimes_3 \mathbf{q}_f^i \right] \bar{\mathbf{X}}_i^{-\mathrm{T}} = \bar{\mathbf{X}}_i^{-1} \left[\left(\left(\left(\mathbf{i}_3^i \right)^{\mathrm{T}_{3,4}} \right)^{\mathrm{T}_{1,4}} \otimes_4 \mathbf{q}_f^i \right) \otimes_3 \mathbf{q}_f^i \right] \bar{\mathbf{X}}_i^{-\mathrm{T}} \tag{170}$$

Because $\mathbf{m}_3^i$ is symmetric by construction,

$$\mathbf{m}_3^i = \left(\left(\left(\mathbf{i}_3^i \right)^{\mathrm{T}_{3,4}} \right)^{\mathrm{T}_{1,4}} \otimes_4 \mathbf{q}_f^i \right) \otimes_3 \mathbf{q}_f^i = \left(\left(\mathbf{i}_3^i \right)^{\mathrm{T}_{2,4}} \otimes_4 \mathbf{q}_f^i \right) \otimes_3 \mathbf{q}_f^i = \left(\mathbf{m}_3^i \right)^{\mathrm{T}} \tag{171}$$

Equation (170) becomes:

$$\begin{aligned}\bar{\mathbf{X}}_i^{-1}\mathbf{m}_3^i\bar{\mathbf{X}}_i^{-\mathrm{T}} = \bar{\mathbf{X}}_i^{-1}\left[\left(\left(\mathbf{i}_3^i\right)^{\mathrm{T}_{2,4}} \otimes_4 \mathbf{q}_f^i\right) \otimes_3 \mathbf{q}_f^i\right]\bar{\mathbf{X}}_i^{-\mathrm{T}} = \\ = \left[\left(\bar{\mathbf{X}}_i^{-1}\left(\mathbf{i}_3^i\right)^{\mathrm{T}_{2,4}} \otimes_2 \bar{\mathbf{X}}_i^{-\mathrm{T}}\right) \otimes_4 \mathbf{q}_f^i\right] \otimes_3 \mathbf{q}_f^i = \left(\mathbf{i}_3^{\bar{\mathbf{X}}_i} \otimes_4 \mathbf{q}_f^i\right) \otimes_3 \mathbf{q}_f^i\end{aligned} \tag{172}$$

Except for the flexible states $\mathbf{q}_f^{i\mathrm{T}}$, everything else in block $\mathbf{M}_{rr4}$ is constant and it can be built with products of constant terms and the bi-linear function involving the tensor.

B.2 Blocks $\mathbf{M}_{fr} = \mathbf{M}_{rf}^{\mathbf{T}}$

The first integral $\mathbf{M}_{rf1}$:

$$\mathbf{M}_{rf1} = \int_i \bar{\mathbf{C}}^{\mathrm{T}}\mathbf{A}\bar{\boldsymbol{\varphi}}\mathrm{d}m = \int_i \begin{bmatrix}\mathbf{A}\bar{c}_0\bar{\boldsymbol{\varphi}} \\ \mathbf{A}\bar{c}_1\bar{\boldsymbol{\varphi}} \\ \mathbf{A}\bar{c}_2\bar{\boldsymbol{\varphi}} \\ \mathbf{A}\bar{c}_3\bar{\boldsymbol{\varphi}}\end{bmatrix}\mathrm{d}m \tag{173}$$

The scalar coefficients $\bar{c}_0$, $\bar{c}_j, j = 1,2,3$ multiply each element of $\bar{\boldsymbol{\varphi}} \in \mathbb{R}^{3\times n_f^i}$, then:

$$\int_i \bar{c}_0\bar{\boldsymbol{\varphi}}\mathrm{d}m = \int_i \bar{\boldsymbol{\varphi}}\mathrm{d}m + \left[\int_i \left(\bar{\boldsymbol{\varphi}} \otimes (\bar{\mathbf{r}} - \bar{\mathbf{r}}_0)\right)^{\mathrm{T}_1}\mathrm{d}m\right] \otimes_2 \bar{\mathbf{X}}_i^{-\mathrm{T}}\mathbf{b}_i \tag{174}$$

$$\int_i \bar{c}_j\bar{\boldsymbol{\varphi}}\mathrm{d}m = \left[\int_i \left(\bar{\boldsymbol{\varphi}} \otimes (\bar{\mathbf{r}} - \bar{\mathbf{r}}_0)\right)^{\mathrm{T}_1}\mathrm{d}m\right] \otimes_2 \bar{\mathbf{X}}_i^{-\mathrm{T}}\mathbf{e}_j \tag{175}$$

And,

$$\mathbf{M}_{rf1} = \begin{bmatrix}\mathbf{M}_{rf1}^0 \\ \mathbf{M}_{rf1}^j\end{bmatrix}; j = 1,2,3. \tag{176a}$$

$$\mathbf{M}_{rf1}^0 = \mathbf{A}_i\left(\mathbf{i}_1^i + \mathbf{i}_2^i \otimes_2 \bar{\mathbf{X}}_i^{-\mathrm{T}}\mathbf{b}_i\right) = \left(\mathbf{M}_{rf1}^0\right)_{\mathbf{q}_r^i} \otimes_3 \mathbf{q}_r^i \tag{176b}$$

$$\mathbf{M}_{rf1}^j = \mathbf{A}_i\mathbf{i}_2^i \otimes_2 \bar{\mathbf{X}}_i^{-\mathrm{T}}\mathbf{e}_j = \left(\mathbf{M}_{rf1}^j\right)_{\mathbf{q}_r^i} \otimes_3 \mathbf{q}_r^i \tag{176c}$$

The previous expressions can be expanded by means of (21) and (22).

$$\mathbf{M}_{rf1} = \begin{bmatrix}\mathbf{E} \otimes_2 \mathbf{m}_{rf1}^{00} \;\big|_3\; \mathbf{E} \otimes_2 \mathbf{m}_{rf1}^{0k} \\ \mathbf{E} \otimes_2 \mathbf{m}_{rf1}^{j0} \;\big|_3\; \mathbf{E} \otimes_2 \mathbf{m}_{rf1}^{jk}\end{bmatrix} \otimes_3 \mathbf{q}_r^i = \left(\mathbf{M}_{rf1}\right)_{\mathbf{q}_r^i} \otimes_3 \mathbf{q}_r^i \tag{177a}$$

$$\mathbf{m}_{rf1}^{00} = \mathbf{b}_i^{\mathrm{T}}\left(\mathbf{i}_1^{\bar{\mathbf{X}}_i} + \mathbf{i}_2^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{b}_i\right) = \left(m_{rr2}^{00}\right)_{\mathbf{q}_f} \tag{177b}$$

$$\mathbf{m}_{rf1}^{j0} = \mathbf{b}_i^{\mathrm{T}}\left(\mathbf{i}_2^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{e}_j\right) = \left(m_{rr2}^{j0}\right)_{\mathbf{q}_f} \tag{177c}$$

$$\mathbf{m}_{rf1}^{0k} = \mathbf{e}_k^{\mathrm{T}}\left(\mathbf{i}_1^{\bar{\mathbf{X}}_i} + \mathbf{i}_2^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{b}_i\right) = \left(m_{rr2}^{0k}\right)_{\mathbf{q}_f} \tag{177d}$$

$$\mathbf{m}_{rf1}^{jk} = \mathbf{e}_k^{\mathrm{T}} \left(\mathbf{i}_2^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{e}_j \right) = \left(m_{rr2}^{jk} \right)_{\mathbf{q}_f} \tag{177e}$$

From equations (177), the derivation of $\mathbf{M}_{rf1}$ in section 3.3.2 is straightforward.

The second term $\mathbf{M}_{fr2} = \mathbf{M}_{rf2}^{\mathrm{T}}$, making use of (162):

$$\begin{aligned} \mathbf{M}_{rf2} &= \int_i \left(\mathbf{A}_{\mathbf{q}_r} \otimes_2 \bar{\mathbf{r}}_f \right)^{\mathrm{T}} \mathbf{A} \bar{\boldsymbol{\varphi}} \mathrm{d}m = \\ &= \int_i \left[\left(\bar{\mathbf{r}}_f^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{b} \right) \mathbf{I}_3 \left(\bar{\mathbf{r}}_f^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{e}_1 \right) \mathbf{I}_3 \left(\bar{\mathbf{r}}_f^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{e}_2 \right) \mathbf{I}_3 \left(\bar{\mathbf{r}}_f^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{e}_3 \right) \mathbf{I}_3 \right]^{\mathrm{T}} \mathbf{A} \bar{\boldsymbol{\varphi}} \mathrm{d}m \end{aligned} \tag{178a}$$

The previous integrals can be expressed in terms of $\mathbf{i}_3^i$ by some manipulations and be further expanded by means of equations (5), (21) and (22):

$$\mathbf{A} \left(\bar{\mathbf{r}}_f^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{b} \right) \bar{\boldsymbol{\varphi}} = \left\{ \left[\left(\mathbf{A}_{\mathbf{q}_r} \otimes_2 \left(\bar{\boldsymbol{\varphi}}^{\mathrm{T}} \otimes \bar{\boldsymbol{\varphi}} \right)^{\mathrm{T}_{2,4}} \otimes_2 \bar{\mathbf{X}}^{-\mathrm{T}} \right) \otimes_2 \mathbf{b} \right] \otimes_2 \mathbf{q}_f \right\} \otimes_3 \mathbf{q}_r \tag{179}$$

Identically,

$$\mathbf{A} \left(\bar{\mathbf{r}}_f^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{e}_j \right) \bar{\boldsymbol{\varphi}} = \left\{ \left[\mathbf{X}_{\mathbf{q}_r} \otimes_2 \left(\bar{\mathbf{X}}^{-1} \left(\bar{\boldsymbol{\varphi}}^{\mathrm{T}} \otimes \bar{\boldsymbol{\varphi}} \right)^{\mathrm{T}_{2,4}} \otimes_2 \bar{\mathbf{X}}^{-\mathrm{T}} \right) \otimes_2 \mathbf{e}_j \right] \otimes_2 \mathbf{q}_f \right\} \otimes_3 \mathbf{q}_r \tag{180}$$

Then,

$$\mathbf{M}_{rf2} = \begin{bmatrix} \mathbf{M}_{rf2}^0 \\ \mathbf{M}_{rf2}^j \end{bmatrix}; \; j = 1, 2, 3. \tag{181}$$

$$\mathbf{M}_{rf2}^0 = \int_i \mathbf{A} \left(\bar{\mathbf{r}}_f^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{b} \right) \bar{\boldsymbol{\varphi}} \mathrm{d}m = \left[\left(\mathbf{X}_i \right)_{\mathbf{q}_r^i} \otimes_2 \left(\mathbf{i}_3^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{b}_i \right) \otimes_2 \mathbf{q}_f^i \right] \otimes_3 \mathbf{q}_r^i \tag{182}$$

$$\mathbf{M}_{rf2}^j = \int_i \mathbf{A} \left(\bar{\mathbf{r}}_f^{\mathrm{T}} \bar{\mathbf{X}}^{-\mathrm{T}} \mathbf{e}_j \right) \bar{\boldsymbol{\varphi}} \mathrm{d}m = \left[\left(\mathbf{X}_i \right)_{\mathbf{q}_r^i} \otimes_2 \left(\mathbf{i}_3^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{e}_j \right) \otimes_2 \mathbf{q}_f^i \right] \otimes_3 \mathbf{q}_r^i \tag{183}$$

Equation (181) can be further expanded by means of equation (22):

$$\mathbf{M}_{rf2} = \left(\begin{bmatrix} \mathbf{E} \otimes_2 \mathbf{M}_{rf2}^{00} \Big|_4 \mathbf{E} \otimes_2 \mathbf{M}_{rf2}^{0k} \\ \mathbf{E} \otimes_2 \mathbf{M}_{rf2}^{j0} \Big|_4 \mathbf{E} \otimes_2 \mathbf{M}_{rf2}^{jk} \end{bmatrix} \otimes_2 \mathbf{q}_f^i \right) \otimes_3 \mathbf{q}_r^i; \; j, k = 1, 2, 3. \tag{184a}$$

$$\mathbf{M}_{rf2}^{00} = \mathbf{b}_i^{\mathrm{T}} \left(\mathbf{i}_3^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{b}_i \right) = \mathbf{T}_{rr4}^{00} \tag{184b}$$

$$\mathbf{M}_{rf2}^{j0} = \mathbf{b}_i^{\mathrm{T}} \left(\mathbf{i}_3^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{e}_j \right) = \mathbf{e}_j^{\mathrm{T}} \mathbf{T}_{rr4}^{\mathbf{3}0} = \mathbf{T}_{rr4}^{j0} = \mathbf{T}_{rr4}^{0j} \tag{184c}$$

$$\mathbf{M}_{rf2}^{0k} = \mathbf{e}_k^{\mathrm{T}} \left(\mathbf{i}_3^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{b}_i \right) = \mathbf{e}_k^{\mathrm{T}} \mathbf{T}_{rr4}^{0\mathbf{3}} = \mathbf{T}_{rr4}^{0k} = \mathbf{T}_{rr4}^{k0} \tag{184d}$$

$$\mathbf{M}_{rf2}^{jk} = \mathbf{e}_k^{\mathrm{T}} \left(\mathbf{i}_3^{\bar{\mathbf{X}}_i} \otimes_2 \mathbf{e}_j \right) \tag{184e}$$

Observe that the same constant terms appearing in (169) are also present here. Equations in section 3.3.2 are straightforward from (184).

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