Adjoint Sensitivity Analysis of Multibody System Equations in State-Space Representation obtained by QR Decomposition

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EXTENDED ABSTRACT

1 Introduction

Gradient determination is an important step in the analysis and optimization of rigid and flexible multibody systems. If the number of design variables is high, the adjoint variable method is often the most efficient approach to sensitivity analysis. However, a set of adjoint differential equations have to be derived and solved first, whose structure depends on the structure of the multibody system equations. In general, the system equations can be formulated in implicit differential-algebraic form as

$$\begin{aligned}
\mathbf{x} \in \mathbb{R}^h \quad & \text{design variables} \\
\mathbf{z}_\mathrm{I}(t,\mathbf{x}), \mathbf{z}_\mathrm{II}(t,\mathbf{x}) \in \mathbb{R}^r \quad & \text{redundant position and velocity variables} \\
\boldsymbol{\lambda}(t,\mathbf{x}) \in \mathbb{R}^{n_\mathrm{c}} \quad & \text{Lagrange multipliers} \\
\boldsymbol{\phi}^0(t^0, \mathbf{z}_\mathrm{I}^0, \mathbf{x}) = \mathbf{0} \quad & \text{initial conditions (position level)} \\
\dot{\boldsymbol{\phi}}^0(t^0, \mathbf{z}_\mathrm{I}^0, \mathbf{z}_\mathrm{II}^0, \mathbf{x}) = \mathbf{0} \quad & \text{initial conditions (velocity level)} \\
\dot{\mathbf{z}}_\mathrm{I} - \mathbf{Z}(\mathbf{z}_\mathrm{I})\mathbf{z}_\mathrm{II} = \mathbf{0} \quad & \text{kinematic relation} \\
\mathbf{M}(\mathbf{z}_\mathrm{I},\mathbf{x})\dot{\mathbf{z}} - \mathbf{f}(t,\mathbf{z}_\mathrm{I},\mathbf{z}_\mathrm{II},\mathbf{x}) - \mathbf{C}^\mathsf{T}(\mathbf{z}_\mathrm{I},\mathbf{x})\boldsymbol{\lambda} = \mathbf{0} \quad & \text{kinetic equations} \\
\mathbf{c}(t,\mathbf{z}_\mathrm{I},\mathbf{x}) = \mathbf{0} \quad & \text{constraint equations (position level)}
\end{aligned} \tag{1}$$

whereby $\mathbf{Z}$ is the kinematic matrix, $\mathbf{M}$ the global mass matrix, $\mathbf{f}$ comprises the generalized inertia forces, elastic forces, and the applied loads, and $\mathbf{C}$ is the Jacobian matrix of the constraint equations $\mathbf{c}$. Since the numerical solution of this index-3 system is demanding, the index is often reduced by differentiating the kinematic constraints twice

$$\dot{\mathbf{c}}(t,\mathbf{z}_\mathrm{I},\mathbf{z}_\mathrm{II},\mathbf{x}) = \underbrace{\frac{\partial \mathbf{c}}{\partial \mathbf{z}_\mathrm{I}}}_{\mathbf{C}}\mathbf{Z}\mathbf{z}_\mathrm{II} + \underbrace{\frac{\partial \mathbf{c}}{\partial t}}_{\mathbf{c}_\mathrm{t}} = \mathbf{0}, \quad \ddot{\mathbf{c}}(t,\mathbf{z}_\mathrm{I},\mathbf{z}_\mathrm{II},\mathbf{x}) = \mathbf{C}\dot{\mathbf{z}}_\mathrm{II} + \underbrace{\dot{\mathbf{C}}\mathbf{z}_\mathrm{II} + \frac{\partial^2 \mathbf{c}}{\partial t^2}}_{\mathbf{c}_\mathrm{tt}} = \mathbf{0}, \tag{2}$$

and considering the constraints at acceleration level in the time integration.

2 Projection of System Equations

Alternatively to the index reduction, the system equations (1) can be transformed into a set of f ordinary differential equations (ODEs) by, for instance, a projection as in [3] before deriving the adjoint sensitivity equations. While the projectors in [3] are determined from a manual coordinate partitioning, in this work, a full QR decomposition [2] is used. From the Jacobian of the constraints $\mathbf{C}$, two orthogonal matrices can be determined as

$$\mathbf{C}^\mathsf{T} = \mathbf{Q}\mathbf{R} = \begin{bmatrix}\mathbf{Q}_1 & \mathbf{Q}_2\end{bmatrix}\begin{bmatrix}\mathbf{R}_1 \\ \mathbf{0}\end{bmatrix}, \quad \mathbf{Q}_1 \in \mathbb{R}^{r\times n_\mathrm{c}}, \mathbf{Q}_2 \in \mathbb{R}^{r\times f}, \mathbf{R}_1 \in \mathbb{R}^{n_\mathrm{c}\times n_\mathrm{c}}, \tag{3}$$

which represent the constrained and free motion directions $\mathbf{Q}_1$ and $\mathbf{Q}_2$ of the multibody system. Accordingly, the redundant velocity and acceleration coordinates can be split as

$$\mathbf{z}_\mathrm{II} = \mathbf{Q}_2\mathbf{z} + \mathbf{Q}_1\bar{\mathbf{z}}, \quad \dot{\mathbf{z}}_\mathrm{II} = \mathbf{Q}_2\mathbf{a} + \mathbf{Q}_1\bar{\mathbf{a}}, \tag{4}$$

into independent and dependent coordinates $\mathbf{z}, \mathbf{a} \in \mathbb{R}^f$, and $\bar{\mathbf{z}}, \bar{\mathbf{a}} \in \mathbb{R}^{n_\mathrm{c}}$, respectively. The latter can be determined from the constraint equations at velocity and acceleration level (2) as

$$\bar{\mathbf{z}} = -\left(\mathbf{C}\mathbf{Q}_1\right)^{-1}\left(\mathbf{C}\mathbf{Q}_2\mathbf{z} + \mathbf{c}_\mathrm{t}\right) \quad \text{and} \quad \bar{\mathbf{a}} = -\left(\mathbf{C}\mathbf{Q}_1\right)^{-1}\left(\mathbf{C}\mathbf{Q}_2\mathbf{a} + \mathbf{c}_\mathrm{tt}\right), \tag{5}$$

whereby $\mathbf{C}\mathbf{Q}_1 = \mathbf{R}_1^\mathsf{T}$ and $\mathbf{C}\mathbf{Q}_2 = \mathbf{0}$. Using Eq. (5) to substitute the dependent velocities and accelerations in Eq. (4) yields

$$\mathbf{z}_\mathrm{II} = \mathbf{Q}_2\mathbf{z} - \mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}}\mathbf{c}_\mathrm{t}, \tag{6a}$$

$$\dot{\mathbf{z}}_\mathrm{II} = \mathbf{Q}_2\mathbf{a} - \mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}}\mathbf{c}_\mathrm{tt}. \tag{6b}$$

Plugging Eq. (6a) in into the kinematic relation of the system equations (1) gives

$$\dot{\mathbf{z}}_{\mathrm{I}} - \mathbf{Z}\left(\mathbf{Q}_2\mathbf{z} - \mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}}\mathbf{c}_{\mathrm{t}}\right) = \mathbf{0}. \tag{7}$$

Moreover, the variation $\delta\mathbf{z}_{\mathrm{II}} = \mathbf{Q}_2\delta\mathbf{z}$ of Eq. (6a), and Eq. (6b) are plugged in into Jourdain's principle of mechanics yielding

$$\delta\mathbf{z}^{\mathsf{T}}\mathbf{Q}_2^{\mathsf{T}}\left\{\mathbf{M}\left(\mathbf{Q}_2\mathbf{a} - \mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}}\mathbf{c}_{\mathrm{tt}}\right) - \mathbf{C}^{\mathsf{T}}\boldsymbol{\lambda} - \mathbf{f}\right\} = 0, \quad \forall\delta\mathbf{z}. \tag{8}$$

Since $\mathbf{Q}_2^{\mathsf{T}}\mathbf{C}^{\mathsf{T}} = \mathbf{0}$, the reaction forces in Eq. (8) vanish and the minimal accelerations $\mathbf{a}$ can be determined as

$$\mathbf{a} = \left(\mathbf{Q}_2^{\mathsf{T}}\mathbf{M}\mathbf{Q}_2\right)^{-1}\left(\mathbf{Q}_2^{\mathsf{T}}\mathbf{M}\mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}}\mathbf{c}_{\mathrm{tt}} + \mathbf{Q}_2^{\mathsf{T}}\mathbf{f}\right). \tag{9}$$

Equation (7) and Eq. (6b), in which the minimal accelerations (9) are incorporated, represent the multibody system in state-space formulation and can be summarized as follows

$$\begin{aligned}
\dot{\mathbf{z}}_{\mathrm{I}} &= \mathbf{v}(t, \mathbf{z}_{\mathrm{I}}, \mathbf{z}_{\mathrm{II}}, \mathbf{x}) = \mathbf{Z}\left(\mathbf{Q}_2\mathbf{Q}_2^{\mathsf{T}}\mathbf{z}_{\mathrm{II}} - \mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}}\mathbf{c}_{\mathrm{t}}\right), \\
\dot{\mathbf{z}}_{\mathrm{II}} &= \mathbf{w}(t, \mathbf{z}_{\mathrm{I}}, \mathbf{z}_{\mathrm{II}}, \mathbf{x}) = \mathbf{Q}_2\left(\mathbf{Q}_2^{\mathsf{T}}\mathbf{M}\mathbf{Q}_2\right)^{-1}\left(\mathbf{Q}_2^{\mathsf{T}}\mathbf{M}\mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}}\mathbf{c}_{\mathrm{tt}} + \mathbf{Q}_2^{\mathsf{T}}\mathbf{f}\right) - \mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}}\mathbf{c}_{\mathrm{tt}}.
\end{aligned} \tag{10}$$

It is worth mentioning that the minimal velocities $\mathbf{z}$ are expressed in terms of the redundant velocities $\mathbf{z}_{\mathrm{II}}$. The relation $\mathbf{z} = \mathbf{Q}_2^{\mathsf{T}}\mathbf{z}_{\mathrm{II}}$ is found by multiplying Eq. (4) from the left with $\mathbf{Q}_2^{\mathsf{T}}$ and exploiting $\mathbf{Q}_2^{\mathsf{T}}\mathbf{Q}_2 = \mathbf{I}$ and $\mathbf{Q}_2^{\mathsf{T}}\mathbf{Q}_1 = \mathbf{0}$.

3 Adjoint Differential Equations

The performance of the dynamic system (10) shall be assessed with the comparatively simple but general integral criterion function

$$\psi(\mathbf{x}) = \int_{t^0}^{t^1} F(t, \mathbf{z}_{\mathrm{I}}, \mathbf{z}_{\mathrm{II}}, \dot{\mathbf{z}}_{\mathrm{II}}.\mathbf{x})\mathrm{d}t. \tag{11}$$

To determine the gradient $\nabla\psi = \mathrm{d}\psi/\mathrm{d}\mathbf{x}$ with the adjoint variable method, among others, the system of adjoint differential equations

$$\dot{\mu} = -\left(\frac{\partial\mathbf{v}}{\partial\mathbf{z}_{\mathrm{I}}}\right)^{\mathsf{T}}\mu - \left(\frac{\partial\mathbf{w}}{\partial\mathbf{z}_{\mathrm{I}}}\right)^{\mathsf{T}}\left(\nu + \frac{\partial F}{\partial\dot{\mathbf{z}}_{\mathrm{II}}}\right) - \frac{\partial F}{\partial\mathbf{z}_{\mathrm{I}}}, \quad \dot{\nu} = -\left(\frac{\partial\mathbf{v}}{\partial\mathbf{z}_{\mathrm{II}}}\right)^{\mathsf{T}}\mu - \left(\frac{\partial\mathbf{w}}{\partial\mathbf{z}_{\mathrm{II}}}\right)^{\mathsf{T}}\left(\nu + \frac{\partial F}{\partial\dot{\mathbf{z}}_{\mathrm{II}}}\right) - \frac{\partial F}{\partial\mathbf{z}_{\mathrm{II}}}. \tag{12}$$

have to be set up and solved for the adjoint variables μ and ν. Therefore, as can be seen from Eq. (12), the derivatives of the kinematic and kinetic function $\mathbf{v}$ and $\mathbf{w}$ with respect to the redundant position and velocity coordinates $\mathbf{z}_{\mathrm{I}}$ and $\mathbf{z}_{\mathrm{II}}$ are required to set up the adjoint system. Thus, in contrast to existing formulations [1, 3, 4], the derivatives of $\mathbf{Q}_2$ and $\mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}}$ with respect to the redundant position variables $z_{\mathrm{I}j}, j = 1(1)r$ have to be additionally provided.

There are two ways to determine these derivatives. On the one hand, the derivatives of $\mathbf{Q}_1$, $\mathbf{Q}_2$, and $\mathbf{R}_1$ with respect to $z_{\mathrm{I}j}$ are determined by direct or numerical differentiation of the QR decomposition algorithm. On the other hand, it is possible to derive a set of linear equations to compute the derivatives of $\mathbf{Q}_2$ and $\mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}}$ from Eq. (3) and the orthogonality conditions $\mathbf{Q}_1^{\mathsf{T}}\mathbf{Q}_2 = \mathbf{C}\mathbf{Q}_2 = \mathbf{0}$ such that

$$\begin{aligned}
\frac{\partial\mathbf{Q}_2}{\partial z_{\mathrm{I}j}} &= -\mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}}\frac{\partial\mathbf{C}}{\partial z_{\mathrm{I}j}}\mathbf{Q}_2, \\
\begin{bmatrix}\mathbf{C} \\ \mathbf{Q}_2^{\mathsf{T}}\end{bmatrix}\frac{\partial\left(\mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}}\right)}{\partial z_{\mathrm{I}j}} &= -\begin{bmatrix}\dfrac{\partial\mathbf{C}}{\partial z_{\mathrm{I}j}}\mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}} \\ \dfrac{\partial\mathbf{Q}_2^{\mathsf{T}}}{\partial z_{\mathrm{I}j}}\mathbf{Q}_1\mathbf{R}_1^{-\mathsf{T}}\end{bmatrix}.
\end{aligned} \tag{13}$$

In this work, both approaches are compared with respect to the precision and computational costs in the adjoint sensitivity analysis of rigid and flexible multibody systems. As application examples, a rigid spring pendulum and a flexible slider-crank mechanism modeled with the floating frame of reference formulation are presented.

References

[1] D. Bestle, P. Eberhard. Analyzing and optimizing multibody systems. Mechanics of structures and machines, 20(1), 67-92, 1992.

[2] S. S. Kim, M. J. Vanderploeg. QR decomposition for state space representation of constrained mechanical dynamic systems, Journal of Mechanisms, Transmissions, and Automation in Design, 1986.

[3] D. Dopico, Y. Zhu, A. Sandu, C. Sandu. Direct and adjoint sensitivity analysis of ordinary differential equation multibody formulations. Journal of Computational and Nonlinear Dynamics, 10(1), 2015.

[4] A. Azari Nejat, A. Moghadasi, A. Held. Adjoint sensitivity analysis of flexible multibody systems in differential-algebraic form. Computers & Structures, 2020.