Discrete Adjoint Approach for the Sensitivity Analysis of an Augmented Lagrangian Index-3 Formulation with Projections

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EXTENDED ABSTRACT

1 Introduction

Different mechanical applications, as optimal control and design optimization, require the evaluation of the impact of different parameters in the response of a mechanical system. This variation can be measured through a sensitivity analysis.

The sensitivity analysis of the dynamics of multibody systems can be computed with different methods, from the simplest finite differences to the more complex analytical methods involving direct differentiation [1, 2] or the adjoint variable method [3]. In a sensitivity analysis, three key properties of the calculation must be considered: the accuracy, the computational time and the generality of the expressions for any multibody system. Some calculations like finite differences, could give poorly accurate solutions involving a high consumption of computational time, especially with a large set of parameters. On the other hand, analytical calculations are usually faster and more accurate, but a generalization is not always easy to implement.

The analytical sensitivities can be focused from two different points of view: the forward sensitivity calculations, for which the derivatives of the states must be calculated through the direct differentiation of the expressions of the dynamics; and the adjoint variable method, which only requires to calculate a set of new variables, namely, the adjoint variables.

Recently, the adjoint sensitivity analysis of an augmented Lagrange index-3 formulation with velocity and acceleration projections was developed in [3], considering the equations of motion as continuous in time. The continuous approach constitutes a general method to compute the sensitivity analysis of a multibody system, but it has as main drawbacks the complexity of the initialization of the adjoint variables and the presence of time derivatives of the mass and projection matrices.

In this work, a different approach based on the use of the discrete derivatives of the equations of motion to build the adjoint system of the augmented Lagrange index-3 formulation with projections is developed and tested in a benchmark model (five-bar). The computation of the discrete analytical approach has been implemented in the multibody system library MBSLIM for natural coordinates models.

2 Problem statement

Let us consider a multibody system modeled with $\mathbf{q} \in \mathbb{R}^n$ dependent natural coordinates related by $\mathbf{\Phi} \in \mathbb{R}^m$ holonomic constraints. Applying the ALI3-P scheme, the following equations of motion are achieved:

$$\mathbf{M}\ddot{\mathbf{q}}^* + \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}} \left(\boldsymbol{\lambda}^{*(i+1)} + \boldsymbol{\alpha}\mathbf{\Phi} \right) = \mathbf{Q}, \tag{1}$$

$$\boldsymbol{\lambda}^{*(i+1)} = \boldsymbol{\lambda}^{*(i)} + \boldsymbol{\alpha}\mathbf{\Phi};\, i > 0, \tag{2}$$

where $\mathbf{M} \in \mathbb{R}^{n\times n}$ is the mass matrix of the system, $\mathbf{\Phi}_{\mathbf{q}} \in \mathbb{R}^{m\times n}$ is the jacobian matrix of the constraints, $\mathbf{Q} \in \mathbb{R}^n$ is the vector of generalized forces and $\boldsymbol{\lambda}^* \in \mathbb{R}^m$ the Lagrange multipliers.

In this formulation, the fulfillment of the constraints in velocities and accelerations is imposed with velocity and acceleration projections:

$$\left(\bar{\mathbf{P}} + \varsigma \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}} \boldsymbol{\alpha} \mathbf{\Phi}_{\mathbf{q}}\right) \dot{\mathbf{q}} = \bar{\mathbf{P}}\dot{\mathbf{q}}^* - \varsigma \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}} \boldsymbol{\alpha} \mathbf{\Phi}_t\,, \tag{3}$$

$$\left(\bar{\mathbf{P}} + \varsigma \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}} \boldsymbol{\alpha} \mathbf{\Phi}_{\mathbf{q}}\right) \ddot{\mathbf{q}} = \bar{\mathbf{P}}\ddot{\mathbf{q}}^* - \varsigma \mathbf{\Phi}_{\mathbf{q}}^{\mathrm{T}} \boldsymbol{\alpha} \left(\dot{\mathbf{\Phi}}_{\mathbf{q}}\dot{\mathbf{q}} + \dot{\mathbf{\Phi}}_t\right)\,, \tag{4}$$

where $\bar{\mathbf{P}}$ is a symmetric projection matrix, and the superscript * indicates that the correspondent term is an unprojected magnitude.

Let us consider an objective function expressed as an integral in time:

$$\psi = \int_{t_0}^{t_F} g\left(\mathbf{q}, \dot{\mathbf{q}}, \ddot{\mathbf{q}}, \boldsymbol{\lambda}, \boldsymbol{\rho}\right) \mathrm{dt}. \tag{5}$$

The sensitivity analysis of the objective function with respect to a set of parameters $\boldsymbol{\rho} \in \mathbb{R}^p$ can be computed applying the adjoint method to the objective function using the equations solved in the dynamics, leading to the following Lagrangian:

$$\begin{aligned}\mathscr{L} = \psi - \int_{t_0}^{t_F} \boldsymbol{\mu}^{\mathrm{T}} \left(\mathbf{M}\ddot{\mathbf{q}}^* + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}} \left(\boldsymbol{\lambda}^* + \boldsymbol{\alpha}\boldsymbol{\Phi} \right) - \mathbf{Q} \right) \mathrm{d}t - \int_{t_0}^{t_F} \boldsymbol{\mu}_{\boldsymbol{\Phi}}^{\mathrm{T}} \boldsymbol{\Phi} \mathrm{d}t \\ - \int_{t_0}^{t_F} \boldsymbol{\mu}_{\dot{\boldsymbol{\Phi}}}^{\mathrm{T}} \left(\left[\bar{\mathbf{P}} + \varsigma \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}} \boldsymbol{\alpha} \boldsymbol{\Phi}_{\mathbf{q}} \right] \dot{\mathbf{q}} - \bar{\mathbf{P}} \dot{\mathbf{q}}^* + \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}} \varsigma \boldsymbol{\alpha} \boldsymbol{\Phi}_t \right) \mathrm{d}t - \int_{t_0}^{t_F} \boldsymbol{\mu}_{\ddot{\boldsymbol{\Phi}}}^{\mathrm{T}} \left(\left[\bar{\mathbf{P}} + \varsigma \boldsymbol{\Phi}_{\mathbf{q}}^{\mathrm{T}} \boldsymbol{\alpha} \boldsymbol{\Phi}_{\mathbf{q}} \right] \ddot{\mathbf{q}} - \bar{\mathbf{P}} \ddot{\mathbf{q}}^* + \boldsymbol{\Phi}_{\mathbf{q}} \varsigma \boldsymbol{\alpha} \left(\dot{\boldsymbol{\Phi}}_{\mathbf{q}} \dot{\mathbf{q}} + \dot{\boldsymbol{\Phi}}_t \right) \right) \mathrm{d}t.\end{aligned} \tag{6}$$

Observe that an index-3 formulation was used in the adjoint instead of the augmented Lagrange index-3 in order to avoid the Lagrange multipliers iterations, thanks to the lemma 4.3 presented in [3]. The resulting Lagrangian has 4 arrays of adjoint variables, correspondent to the index-3 part of the dynamics ($\boldsymbol{\mu}$ and $\boldsymbol{\mu}_{\boldsymbol{\Phi}}$), and to the projections of velocities ($\boldsymbol{\mu}_{\dot{\boldsymbol{\Phi}}}$) and accelerations ($\boldsymbol{\mu}_{\ddot{\boldsymbol{\Phi}}}$).

The main change with respect to the continuous approach consists in the use of the discrete derivatives of the previous Lagrangian, applying a numerical integrator in order to express $\dot{\mathbf{q}}^*$ and $\ddot{\mathbf{q}}^*$ in terms of $\mathbf{q}$. This process eludes the integration by parts used in [3] which entails the addition of new terms at times t_0 and t_F and which complicates the initialization of the adjoint variables. The application of the integrator expressions instead of an integration by parts has, however, as bigger drawback the appearance of these integrator expressions in the final adjoint equations.

The discrete adjoint equations are reached by means of considering subsequent steps of time and nullifying the terms multiplying the unknown sensitivities of the states generated during the derivation of (6). In this approach, instead of time integration of variables, an accumulative term from time t_i to time t_{i-1} appears, working as linkage among consecutive instants of time.

The non-existence of dynamic equations further than time t_F allows a much simpler initialization of all the adjoint variables than the continuous approach, with the only need of nullifying the accumulation terms previously commented. The same equations of any instant of time are used in this initialization process.

3 Numerical experiments

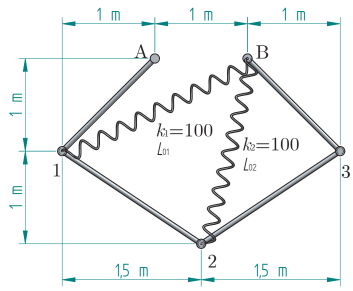

Figure 1: Five-bar mechanism

The test case solved in this work is the five-bar mechanism of Fig. 1 described in [4, 5], with the coefficients of two external actuator torques applied on the joints of the two bars attached to the fixed bar as sensitivity parameters, and with an objective function describing the error between the trajectory described by point $\mathbf{r}_2$ and a reference set of values. This problem is presented as an optimal control test.

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References

[1] D. Dopico, F. González, M. Saura, D. G. Vallejo. Forward sensitivity analysis of the index-3 augmented lagrangian formulation with projections. In Proceeding of the 8th ECCOMAS Thematic Conference on Multibody Dynamics. 2017.

[2] D. Dopico, F. González, A. Luaces, M. Saura, D. García-Vallejo. Direct sensitivity analysis of multibody systems with holonomic and nonholonomic constraints via an index-3 augmented lagrangian formulation with projections. Nonlinear Dynamics, 2018. doi:10.1007/s11071-018-4306-y.

[3] D. Dopico, A. Sandu, C. Sandu. Adjoint sensitivity index-3 augmented lagrangian formulationwith projections. Mechanics Based Design of Structures and Machines, 2021. doi:10.1080/15397734.2021.1890614.

[4] 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):1–8, 2014. doi:10.1115/1.4026492.

[5] D. Dopico, A. Sandu, C. Sandu, Y. Zhu. Sensitivity Analysis of Multibody Dynamic Systems Modeled by ODEs and DAEs., chapter 1, 1–32. Multibody Dynamics - Computational Methods and Applications. Springer, 2014. doi:10.1007/978-3-319-07260-9.