Discrete Adjoint Variable Method Applied to Semi-recursive Augmented Lagrangian Index-3 formulations with projections

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Abstract: *Optimization problems involving a large number of parameters usually require a special treatment of gradient evaluations. The high computational cost of direct differentiation methods (DDM) is commonly reduced by the reformulation of the sensitivity problem by means of the addition of a set of adjoint variables. This work discusses the application of the discrete adjoint variable method (DAVM) to the semi-recursive augmented Lagrangian Index-3 formulation with velocity and acceleration projections recently reviewed in [1]. The resulting sensitivity formulation is tested in a five-bar benchmark problem and in a vehicle model with articulated suspensions.*

Introduction

Numerical experiments demonstrate that optimization methods based on the derivatives of the objective function usually deliver better performance than others based on the sole evaluation of the value of the objective function [2]. The behavior of these so called gradient-based optimization algorithms is strongly tied to the properties of the gradient evaluation method, specially in what is referred to accuracy and CPU time.

The adjoint variable method (AVM) is usually employed in sensitivity analyses which involve a large number of parameters. This method dodges the evaluation of the state sensitivities by means of the addition of a set of adjoint variables, whose dimensions depend on the number of objective functions instead of the number of parameters.

If the equations of motion (EoM) are given by a set of second order differential-algebraic equations (DAE) and they are considered as continuous expressions in time, the generation of the adjoint equations requires a series of transformations, such as an integration by parts, that might lead to high order time derivatives of dynamic magnitudes or to complex initialization processes that require the addition of new conditions and adjoint variables [3]. The DAVM regards the EoM as a set of discrete algebraic equations, which leads to simpler expressions and more direct sensitivity algorithms. As a drawback, the set of equations generated depends on the numerical integrator used to solve the dynamics, which limits its generality.

Semi-recursive ALI3-P formulation

The semi-recursive Augmented Lagrangian Index-3 Formulation with velocity and acceleration projections (ALI3-P) [1] is a robust, accurate and computationally efficient formulation for the evaluation of multibody dynamics. It is based on the solution of an iterative augmented Lagrange index-3 problem:

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

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

followed by velocity and acceleration projections

$$\left(\bar{\mathbf{P}}+\varsigma\boldsymbol{\Phi}_{\hat{\mathbf{z}}}^{\mathrm{T}}\boldsymbol{\alpha}\boldsymbol{\Phi}_{\hat{\mathbf{z}}}\right)\dot{\mathbf{z}}=\bar{\mathbf{P}}\dot{\mathbf{z}}^{*}-\boldsymbol{\Phi}_{\hat{\mathbf{z}}}^{\mathrm{T}}\varsigma\boldsymbol{\alpha}\boldsymbol{\Phi}_{t} \tag{2a}$$

$$\left(\bar{\mathbf{P}}+\varsigma\boldsymbol{\Phi}_{\hat{\mathbf{z}}}^{\mathrm{T}}\boldsymbol{\alpha}\boldsymbol{\Phi}_{\hat{\mathbf{z}}}\right)\ddot{\mathbf{z}}=\bar{\mathbf{P}}\ddot{\mathbf{z}}^{*}-\boldsymbol{\Phi}_{\hat{\mathbf{z}}}^{\mathrm{T}}\varsigma\boldsymbol{\alpha}\left(\dot{\boldsymbol{\Phi}}_{\hat{\mathbf{z}}}\dot{\mathbf{z}}+\dot{\boldsymbol{\Phi}}_{t}\right) \tag{2b}$$

in which $\mathrm{M}(\mathbf{z},\boldsymbol{\rho})\in\mathbb{R}^{n\times n}$ is the mass matrix, $\ddot{\mathbf{z}}^{*}\in\mathbb{R}^{n}$ the unprojected velocities, $\boldsymbol{\Phi}_{\hat{\mathbf{z}}}(\mathbf{z},\boldsymbol{\rho})\in\mathbb{R}^{m\times n}$ is the Jacobian of the constraints, $\boldsymbol{\lambda}^{*}\in\mathbb{R}^{m}$ corresponds to the approximate Lagrange multipliers, $\boldsymbol{\alpha}\in\mathbb{R}^{m\times m}$ is a diagonal penalty matrix, $\mathbf{Q}(\mathbf{z},\dot{\mathbf{z}}^{*},\boldsymbol{\rho})\in\mathbb{R}^{n}$ is the vector of generalized forces and the superindex i indicates the iteration index. Regarding the projections, $\bar{\mathbf{P}}\in\mathbb{R}^{n\times n}$ is a symmetric projection matrix and ς is a penalty factor.

DAVM method

The application of the DAVM to semi-recursive ALI3-P formulations begins with the definition of the following instant Lagrangian:

$$\begin{aligned}\mathcal{L}_{i}=\boldsymbol{\psi}-\boldsymbol{\mu}_{\ddot{\boldsymbol{\Phi}}}^{\mathrm{T}}\left(\left[\bar{\mathbf{P}}+\varsigma\boldsymbol{\Phi}_{\hat{\mathbf{z}}}^{\mathrm{T}}\boldsymbol{\alpha}\boldsymbol{\Phi}_{\hat{\mathbf{z}}}\right]\ddot{\mathbf{z}}-\bar{\mathbf{P}}\ddot{\mathbf{z}}^{*}+\boldsymbol{\Phi}_{\hat{\mathbf{z}}}\varsigma\boldsymbol{\alpha}\left(\dot{\boldsymbol{\Phi}}_{\hat{\mathbf{z}}}\dot{\mathbf{z}}+\dot{\boldsymbol{\Phi}}_{t}\right)\right)-\boldsymbol{\mu}_{\boldsymbol{\Phi}}^{\mathrm{T}}\boldsymbol{\Phi}\\-\boldsymbol{\mu}^{\mathrm{T}}\left(\mathrm{M}\ddot{\mathbf{z}}^{*}+\boldsymbol{\Phi}_{\hat{\mathbf{z}}}^{\mathrm{T}}\left(\boldsymbol{\lambda}^{*}+\boldsymbol{\alpha}\boldsymbol{\Phi}\right)-\mathbf{Q}\right)-\boldsymbol{\mu}_{\dot{\boldsymbol{\Phi}}}^{\mathrm{T}}\left(\left[\bar{\mathbf{P}}+\varsigma\boldsymbol{\Phi}_{\hat{\mathbf{z}}}^{\mathrm{T}}\boldsymbol{\alpha}\boldsymbol{\Phi}_{\hat{\mathbf{z}}}\right]\dot{\mathbf{z}}-\bar{\mathbf{P}}\dot{\mathbf{z}}^{*}+\boldsymbol{\Phi}_{\hat{\mathbf{z}}}^{\mathrm{T}}\varsigma\boldsymbol{\alpha}\boldsymbol{\Phi}_{t}\right)\end{aligned} \tag{3}$$

wherein $\boldsymbol{\psi}\in\mathbb{R}^{o}$ is the objective function vector, and $\boldsymbol{\mu},\boldsymbol{\mu}_{\dot{\boldsymbol{\Phi}}},\boldsymbol{\mu}_{\ddot{\boldsymbol{\Phi}}}\in\mathbb{R}^{n\times o}$, $\boldsymbol{\mu}_{\boldsymbol{\Phi}}\in\mathbb{R}^{m\times o}$ are the adjoint variables, being o the number of objective functions, n the number of relative coordinates and m the size of the constraints vector. Taking derivatives on (3) and numerically integrating over time, a new set of adjoint variable equations and a new gradient expression can be obtained.

Numerical experiments

The DAVM applied to semi-recursive ALI3-P formulations has been implemented in the general purpose multibody library MBSLIM. The accuracy of the method has been tested in a five-bar benchmark problem, while its efficiency has been assessed in a more complex model, a four-wheeled vehicle with articulated suspensions. All the results have been compared against other sensitivity formulations.

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