Modeling, Sensitivity Analysis, and Optimization of Hybrid, Constrained Mechanical Systems

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ABSTRACT

This dissertation provides a complete mathematical framework to compute the sensitivities with respect to system parameters for any second order hybrid Ordinary Differential Equation (ODE) and rank 1 and 3 Differential Algebraic Equation (DAE) systems.

The hybrid system is characterized by discontinuities in the velocity state variables due to an impulsive forces at the time of event. At the time of event, such system may also exhibit a change in the equations of motion or in the kinematic constraints.

The analytical methodology that solves the sensitivities for hybrid systems is structured based on jumping conditions for both, the velocity state variables and the sensitivity matrix. The proposed analytical approach is then benchmarked against a known numerical method.

The mathematical framework is extended to compute sensitivities of the states of the model and of the general cost function with respect to model parameters for both, unconstrained and constrained, hybrid mechanical systems.

This dissertation emphasizes the penalty formulation for modeling constrained mechanical systems since this formalism has the advantage that it incorporates the kinematic constraints inside the equation of motion, thus easing the numerical integration, works well with redundant constraints, and avoids kinematic bifurcations.

In addition, this dissertation provides a unified mathematical framework for performing the direct and the adjoint sensitivity analysis for general hybrid systems associated with general cost functions. The mathematical framework computes the jump sensitivity matrix of the direct sensitivities which is found by computing the Jacobian of the jump conditions with respect to sensitivities right before the event. The main idea is then to obtain the transpose of the jump sensitivity matrix to compute the jump conditions for the adjoint sensitivities.

Finally, the methodology developed obtains the sensitivity matrix of cost functions with respect to parameters for general hybrid ODE systems. Such matrix is a key result for design analysis as it provides the parameters that affect the given cost functions the most. Such results could be applied to gradient based algorithms, control optimization, implicit time integration methods, deep learning, etc.

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GENERAL AUDIENCE ABSTRACT

A mechanical system is composed of many different parameters, like the length, weight and inertia of a body or the spring and damping constant of a suspension system. A variation of these constants can modify the motion a mechanical system.

This dissertation provides a complete mathematical framework that aims at identifying the parameters that affect at most the motion of a mechanical system.

Such system could be hybrid like the human body. Indeed, when walking the foot/ground impact causes an abrupt change of velocity of the foot, while the position of the foot remains the same. Such change makes the velocity of the human body to be discontinuous at such event, which makes the human body when walking a hybrid system. The same can be applied to a vehicle driving over a bump.

The main result obtained from the mathematical framework is called the "sensitivity matrix". Such matrix is a key result for design analysis as it identifies the parameters that affect at most the motion of a mechanical system.

Such results are very relevant and could be applied to different softwares with prebuilt gradient based algorithms, control optimization, implicit time integration methods, or deep learning, etc.

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Nomenclature

Dimensions

n	The number of generalized coordinates
p	The number of parameters
k	The number of cost functions
m	The number of equations of constraints

Dynamics

f^{eom}	The function solving the Equation of Motion $\in \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^n$
q, $\dot{q} \in \mathbb{R}^n$	The generalized position and velocity state vector
$\ddot{q} \in \mathbb{R}^n$	The generalized acceleration state vector
$z \in \mathbb{R}^k$	The vector of quadrature variables
$x \in \mathbb{R}^{(2n+p+n_c)}$	The state vector of the canonical ODE
$t_{\text{eve}} \in \mathbb{R}$	The time of event
$\rho \in \mathbb{R}^p$	The vector of system parameters
F	The generalized force vector $\in \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^n$
M	The generalized smooth and invertible Mass matrix $\in \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^{n \times n}$
Φ	The equations of constraints $\in \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^m$

General

$\dot{\square}$ or $\ddot{\square}$	The total (first or second order) derivative of a function or variable with respect to time
$\square_{\zeta,\phi}$	Double subscripts indicates a three-dimensional Jacobian with respect to a quantity ζ and ϕ, unless stated otherwise
$\square_{\zeta}$	Subscript indicates partial derivative with respect to a quantity ζ, unless stated otherwise

Sensitivity Analysis

$Q \in \mathbb{R}^{n\times p}$	The sensitivity matrix of the state vector q with respect to the vector of system parameters ρ
$V \in \mathbb{R}^{n\times p}$	The sensitivity matrix of the state vector $\dot{q}$ with respect to the vector of system parameters ρ
$X \in \mathbb{R}^{(2n+p+n_c)\times p}$	The sensitivity matrix of the x state vector with respect to the vector of system parameters ρ
$dt_{\text{eve}}/d\rho \in \mathbb{R}^{1\times p}$	The sensitivity of the time of event t_{eve} with respect to the vector of system parameters ρ
$\lambda \in \mathbb{R}^{(2n+p+n_c)\times n_c}$	The adjoint sensitivity matrix of X
$\lambda^Q \in \mathbb{R}^{n\times n_c}$	The adjoint sensitivity matrix of Q
$\lambda^V \in \mathbb{R}^{n\times n_c}$	The adjoint sensitivity matrix of V
$\psi \in \mathbb{R}^k$	The vector of cost functions
$g \in \mathbb{R}^k$	The vector of trajectory cost functions
$w \in \mathbb{R}^k$	The vector of terminal cost functions
$Z \in \mathbb{R}^{k\times p}$	The sensitivity matrix of the vector of quadrature variables z

Chapter 1

Introduction And Research Background

1.1 Terminology and History

1.1.1 History

History of the foundation of Classical Mechanics. This dissertation relies on the theoretical foundation of Classical Mechanics that covers a century of mathematical evolution from 1687 to 1788 on dynamic equations of motion for constrained mechanical systems. The foundation starts with Isaac Newton when he presented in 1687 his book “Philosophiae Naturalis Principia Mathematica" [3] that describes the Newton’s Law of motion and of universal gravitation. His theory was based on the work of Galileo Galilee that mathematically described motion of bodies with constant acceleration in his book “The Discourses and Mathematical Demonstrations Relating to Two New Sciences" [4], published in 1638. One of Galileo's most famous scientific experiment was to drop objects of different masses from the leaning tower of Pisa, and to show that they were falling at the same rate. Two main paths dor describing the motion of a body emerged from Newton's foundation: the Newton-Euler equations and the Lagrange's equations of motion. A century after Newton, Euler presented his study on the three dimensional dynamical motion of rigid bodies (translational and rotational motion) that led to his Newton-Euler equations of motion [5]. On the other hand, Jacques Bernoulli worked on systems under static equilibrium in the early eighteenth century, in which he described the principle of virtual work in his letter to Pierre Varignon in 1715. The principle was published ten years latter (in 1725), in Varignon's "Second volume of Nouvelle mecanique ou Statique" [6]. Based on Bernoulli's work, D'Alembert introduced his principle in 1743 that describes the concept of virtual displacements and constraints forces, published in his "Traite de dynamique" [7]. His idea was to implement the concept of virtual work into dynamics problems. Finally, Lagrange synthesized the foundation of classical mechanics by presenting a clear and concise fundamental principle of mechanics, known as Lagrange's equations of motion, presented in 1788 in his "Mechanique Analitique" [8]. Today, his principal is the most well-known and taught to identify the dynamics equation of motion for constrained mechanical systems. For more details on the history of the theoretical foundation of Classical Mechanics, I would recommend the book "History of virtual work laws: a history of mechanics prospective" [9] from Capecchi published in 2012, and the following citations [8, 10, 11, 12].

Multibody dynamics. In this dissertation, a constrained mechanism refers to a constrained rigid multibody dynamic system. According to Jens Wittenburg [13], Schiehlen [14] and Rahnejat [15], well-known researchers in the field of multibody dynamics, Fischer has started the study of multibody dynamics [16]. He established the equation of motion of human walking gait using Euler angles and Lagrange's equation. The multibody dynamics field in the United States has grown thanks to strong strong PhD student-advisor relationship that brought key advances in the field. A few highlights of interest are outlined here:

- Professor Richard S. Hartenberg and his student Jacques Denavit from France (graduated in 1952) published numerous papers and a book [17] on kinematic and dynamic analysis of three dimensional multibody systems. In the early age of digital computers and robotics arms, their formula known as the Denavit–Hartenberg convention has been developed, and it has been widely used since then [18]. This convention transforms local body coordinates to the global reference frame using joints transformations.
- Professor Milton A. Chace and his student Nicolae Orlandea from Romania (graduated in 1972) created the multibody dynamics software package latter known as ADAMS (Automatic Dynamic Analysis of Mechanical Systems). Their method for solving large rigid multibody systems was based on Lagrangian dynamics, sparse matrix techniques, modal optimization, and linearized dynamic equation for implicit integrator [19]. I would recommend the two pages of biography from Dr. Nicolae Orlandea [20] where he provided details on his PHD work that led to the software package ADAM and shared aspects about his professional life and relationships with Dr. Wehage and Dr.

Milton A. Chace. Further details can be found in Dr. Nicolae Orlandeo 's dissertation [21].

- Professor Edward J. Haug and his student Roger Wehage (graduated in 1980) contributed to the coordinate partitioning method for dimension reduction of constrained dynamic systems [22], [23]. Their work led to a minimization of the set of equations of motion by differentiating the dependent and independent velocity variables and excluding constraint reaction forces.

- Professor Roger Wehage and his student Ahmed Shabana from Egypt (graduated in 1982) contributed to the extension of the multibody systems field by moving from the approach of rigid bodies to flexible multibody systems. Poor attention was given in the early eighties to this field and Ahmed Shabana's dissertation provided the mathematical methodology to solve such systems [24]. Details of the history of this field can be found in Dr. Ahmed Shabana's literature review paper [25].

In 2017, the community of multibody dynamics celebrated its forty years of existence. Indeed, the first conference called "Dynamics of multibody systems" was organized by K. Magnus in Berlin in 1977. The conference was sponsored by the International Union of Theoretical and Applied Mechanics (IUTAM).

1.1.2 Terminology

Kinematic Constraints A kinematic constraint establishes a relationship between the state variables of the system (position and velocity). We differentiate between two types of kinematic constraints: bilateral and unilateral. The bilateral constraint refers to a relationship described by an equality equation, while the unilateral constraint refers to a relationship described by an inequality equation. Among the bilateral constraints we differentiate between the holonomic and nonholonomic constraints. As explained in [10] and referred to in Hertz [26], the word holonomic is derived from the Greek words holos, “complete", and nomos, “law", which aims at describing a system configuration made out of interconnected elements governed by a natural law. The difference between Holonomic and nonholonomic constrained systems is that the constraint equations for a Holonomic constrained system are position dependent, while for a nonholonomic constrained system, the constraint equations are position and velocity dependent. Example of a holonomic constrained system is a pendulum in which the two extrema points are constrained by a fixed distance. An example of a nonholonomic system is the rolling disk or ball. Finally, we differentiate between two other types of constraints: the scleronomic and rheonomic constraints. The kinematic constraint equations that are time dependent are referred to as rheonomic, and those that are independent on time are called scleronomic.

Mobility and Type of Coordinates We identify two main approaches in modeling constrained mechanical systems. The first approach aims at reducing the number of state variables by associating each variable with the system's configuration. When modeling an open loop mechanism, such as a robotic arm, the number of state variables is equal to the number of degrees of freedom in the system. The second approach provides the full set of coordinates of each body that composes the multibody system. Each body has 6 degrees of freedom parametrization. Kinematic constraints between bodies are added to restrict their possible movement to a specific subspace. In this study, we use the second approach to model constrained mechanical systems by providing three Cartesian coordinates at the center of gravity and four Euler parameters to define each body's orientation.

Constrained Mechanical Systems. This study deals with kinematic constrained of mechanical systems in which the position, Φ, the velocity, $\dot{\Phi}$, and the acceleration, $\ddot{\Phi}$, constraints given in Eq.3.30 should be satisfied at each time step. The kinematic constraints are assumed to be bilateral, holonomic, and scleronomic.

$$\begin{aligned} \Phi &= \mathsf{0}\ , \\ \dot{\Phi} &= \Phi_q \dot{q} + \Phi_t\, , \\ \ddot{\Phi} &= \Phi_q \ddot{q} + \dot{\Phi}_q \dot{q} + \dot{\Phi}_t \end{aligned} \tag{1.1}$$

Where $\dot{q}$ are the position and the velocity state variables, ρ is the system parameters, the vector of the generalized external forces and Φ_q the Jacobian of the constraints equation Φ.

ODE Model. To satisfy the constraints, this research uses the penalty formulation Eq.1.2 [27] that combines together the kinematic constraints and the equation of motion defined as a second order smooth ODE (Ordinary Differential Equation) system.

$$\begin{aligned}
&\ddot{q} = f^{\text{eom}}(t,\, q,\, v,\, \rho) \\
&f^{\text{eom}} = \overline{\mathsf{M}}^{-1}(t,\, q,\, v,\, \rho)\overline{\mathsf{F}}(t,\, q,\, v,\, \rho), \\
&\overline{\mathsf{M}} = \mathsf{M} + \Phi_q^{\mathrm{T}} \alpha \Phi_q, \\
&\overline{\mathsf{F}} = \mathsf{F} - \Phi_q^{\mathrm{T}} \alpha \left(\dot{\Phi}_q \dot{q} + \dot{\Phi}_t + 2\xi\omega\dot{\Phi} + \omega^2 \Phi \right),
\end{aligned} \tag{1.2}$$

Where $\overline{\mathsf{M}}$ is the generalized mass matrix, and $\overline{\mathsf{F}}$ is the vector of the generalized external forces.

HODE Model. In the context of this dissertation we define a HODE (Hybrid Ordinary Differential Equation) system as a continuous system of second order ODE equations that exhibits discontinuities in the velocity state variables at the time of an event. This event time is referred to as the time of impact as we analyze a mechanical system subjected to instantaneous impact. The impact can be characterized as an impulse in the external forces or a sudden change of configuration constraints.

DAE Model. Differential Algebraic Equations are also explored in this dissertation. The system is defined as index 3 def. 2.3.3 or index 1 def. 2.3.4 when the equation of motion 3.1 is associated with the position or the acceleration constraint equation, respectively.

Sensitivity Analysis and Optimization. The main subject of this dissertation is the sensitivity analysis. When performing design optimization, sensitivity analysis is the first step after the modeling one in which the kinematic and the dynamic analyses are performed. The sensitivity analysis can be performed for any modeling formalism (type of coordinates) and system of equations (ODE and DAE). Sensitivity analysis provides the analytical derivatives of both the response of a system and the associated objective (or cost) function, with respect to the design variables or initial conditions. These derivatives are really relevant for several optimization methods since most of the optimization packages are based on the knowledge of the derivatives. Optimization algorithms use the derivatives to minimize the objective function which is usually associated with the system performance. For example, in vehicle dynamic on objective function is the time integral of the vertical acceleration of the driver during a specific time interval.

1.2 Motivation and Objective

The motivation of the research presented in this dissertation is to provide a clear modeling methodology for dynamic simulations, sensitivity analysis, and optimization of constrained mechanical systems that exhibit impacts. Such systems are among the most complex to conceptualize, understand, and formalized as their study requires accounting for smooth and hybrid trajectories. For example, while walking, the human body is agile and keeps a smooth dynamic equilibrium. When stepping, velocity impacts appear on the foot; a change of constraints is needed when the supported foot is switched. Considering this motivation, I aim at providing a clear methodology and a mathematical framework that would allow any scientist or engineer to run a sensitivity analysis for systems governed by HODE.

This dissertation presents an analytical methodology to compute the sensitivities of the solution of second order hybrid ordinary differential equation (HODE) systems with respect to system parameters. The methodology is extended to the equation of motion for constrained multibody systems.

The analytical methodology resolves the sensitivity with respect to parameters for HODE systems by introducing novel jump conditions for the velocity state variables as well as for the sensitivity variables at the time of impact. The jump conditions for sensitivity analysis at the time of impact relate the interaction of four aspects: the **time**, the **position**, the **velocity**, and the **system parameters**.

To visualize such correlations, we can explore the sensitivity of the governing equations of a free falling ball. The position, the velocity, and the time are related to each other through time integration of the equation of motion. As the ball falls due to its weight, it has a constant acceleration, which is equal to the Earth's gravity. The velocity and the position are found by integrating the acceleration through time. The sensitivity analysis of the free falling ball shows how the position and the velocity of the ball vary with respect to the Earth's gravity. This variation is found by deriving the equation of motion with respect to the Earth's gravity and by integrating it. The time of impact corresponds to the exact time at which the ball impacts the ground. If the value of the Earth's gravity in the equation of motion slightly changes, the time of impact will be different. Thus, this very simple example shows that the time of impact varies with respect to the **time**, the **position**, the **velocity**, and the **system parameters**, and these four variables are dependent on each others. At the time of impact, the position of the ball remains the same, but the ball's velocity is governed by the impulse equation that shifts it to a new value. This sudden velocity jump requires determining the jump of the derivatives of the position and of the velocity with respect to parameters.

The first objective of this dissertation is to provide a unified methodology and a mathematical framework for determining the system's solutions, their direct sensitivities, and sensitivities of a cost function for different types of events. The first type of event is caused by an external impulse (e.g., a contact) leading to a sudden change of velocities. The second type of event is caused by a sudden change of the equations of motion. The third type of event is caused by a sudden change in the kinematic constraints. The dissertation provides new graphical proofs of the jumps in sensitivities at the time of an event, which help better understand the conditions for the jump in the sensitivities. The jump conditions for constrained mechanical systems that are subject to a change in their mechanism and to impulsive forces at the time of event are presented.

The second objective of this study is to provide a unified mathematical framework for performing the direct analysis and the adjoint sensitivity analysis for general hybrid systems associated with general cost functions. The study aims at extending the mathematical framework to handle the non-smoothness of the forward trajectories while performing adjoint sensitivity analysis. The jump sensitivity matrix of the direct sensitivities is built by computing the Jacobian of the jump conditions with respect to sensitivities right before the event. The main idea is then to obtain the transpose of the jump sensitivity matrix to compute the jump conditions for the the adjoint sensitivities.

Finally, this framework facilitates obtaining the sensitivity matrix of cost functions with respect to parameters for general HODE systems. Such matrix is a key result for design analysis as it provides the parameters that affect the given cost functions the most.

All the objectives have been implemented and validated in MATLAB [28] using the symbolic toolbox and also implemented in our in-house modeling, sensitivity analysis, and optimization research software package, MBSVT-FATODE [29].

1.3 Current State-of-the-Art

1.3.1 Sensitivity analysis for smooth systems

Sensitivity analysis plays a key role in a wide range of computational engineering problems, such as design optimization, optimal control, and implicit time integration methods, by providing derivative information for gradient based algorithms and methods. Sensitivity analysis quantifies the effect of small changes in the system parameters onto the outputs of interest [27]. Specifically, in the design of mechanical systems, sensitivity analysis reveals the system parameters that affect the given performance criterion the most, thus providing directions for mechanical design improvements. Sensitivity analysis enables gradient-based optimization by providing the derivative of the cost function with respect to design variables. In adaptive control systems, sensitivity analysis allows assessing the stability of a system by accounting for the effects of system disturbances and system parameters inaccuracies. Applications of sensitivity analysis for control system, such as robotic systems, have been increasing and have become a topic of high interest lately [30, 31].

In this dissertation, the direct and the adjoint sensitivity analysis in the context of ODE and ranked 1 DAE are considered. These approaches are complementary, as the direct sensitivity provides information on how parametric uncertainties propagate through the system dynamics, while the adjoint method is suitable for inverse modeling, in the sense that it can be used to identify the origin of uncertainty in a given model output [32].

Numerical sensitivities are often calculated by finite differences methods, where the deviation of the state trajectories are evaluated after system parameters disturbances or variations in the initial conditions are added in the system. Because of the simplicity of this family of methods, which do not require any additional inputs other than the provided model, they are broadly used. However, finite differences methods are limited to the perturbation size, which may considerably affect the sensitivities [33]. In this dissertation, the analytical direct sensitivity analysis method is investigated and compared to the numerical method.

1.3.2 Sensitivity analysis for hybrid systems

Researches on sensitivity analysis with respect to system parameters and initial conditions for hybrid systems were presented in [34, 35, 36, 37, 38, 39, 40, 41, 42, 43]. The jump conditions of the direct sensitivities for hybrid ODE systems were first presented by Becker [43] in 1966 and a year latter by Rozenvasser [38]. It is thirty years later that Galán *el al.* [35] presented sufficient conditions for the existence and uniqueness of these jump equations. Jump conditions involve the sensitivity of the time of event, and the jumps in the sensitivities of the state variables at the time of event. Within the same period, Hiskens applied them to power switching systems [41]. The jump conditions of the adjoint sensitivities for hybrid ODE systems with discontinuity on the right-hand side and with switching manifold parameters were presented by Stewart in 2010 [44] and Taringoo [45], respectively. Lately, Hong [46] derived the jump conditions for discrete adjoints and applied them on large-scale power systems with switching dynamics. The sensitivity obtained by the adjoint analysis were compared and validated with the forward and finite difference method.

1.3.3 Modeling constrained mechanical systems

The formalism in modeling constrained mechanical system is not unique. Indeed, there is not a unique method in modeling constrained mechanical system that would gather all the researchers in the field of multibody dynamics and robotics. This dissertation does not have the goal of arguing for one formalism and modeling method or another. However, this dissertation has a goal of providing the methodology of sensitivity analysis for hybrid and constrained mechanical systems that can work with any ODE and DAE formalism and modeling method.

To know about all the different formalisms and modeling methods for constrained mechanical systems I would recommend the "Review of Classical Approaches for Constraint Enforcement in Multibody Systems" [47] and "Review of Contemporary Approaches for Constraint Enforcement in Multibody Systems" [48]. Below is the list of well-known methods:

- Maggi's formulation: projection based method of the null space of the Jacobian of the constraints to the equation of motion. The method uses the null space to differentiate between dependent and independent velocity variables. The method was found to be relevant by Dr. Kurdila (1990) [49] and Dr. DeJallon (2012) [50].

- Lagrange's Equations of the First Kind: Differential Algebraic Equations (DAE) method that associates the equations of motion with either the position, the velocity or the acceleration constraint of equations, leading the DAE to be ranked three, two, or one, respectively. Such method suffers from constraint stabilization as only one of the type of constraints is considered.

- Baumgarte's method: a constraint violation stabilization technique that incorporates all the kinematic constraints (position, velocity and the acceleration constraint of equations) into the equation of motion. Dr. P. E. Nikravesh Dr. R. A. Wehage (1985) [51] associated the method with cartesian coordinates at the center of gravity of each body and used Euler parameters for angular orientation. Dr. Park and Dr. Haug associated the method with the generalized coordinate partitioning [52].

- Penalty formulation: a constraint violation stabilization technique that incorporates all the kinematic constraints (position, velocity, and the acceleration constraint equations) into the equation of motion. A first approach of the penalty formulation was presented by Park and Chiou (1988)[53]; the penalty formulation is mentioned by the authors to be more robust and easier to implement that the Baumgarte's method. The full formulation was presented in [54]. Kurdila (1993)[55] showed the convergence and stability of the method. De Jalon and Bayo [56] were in favor on this formulation as the penalty formulation works with redundant constraints and near kinematic singular configurations, whereas the Baumgarte's method fails for such configurations . The reader may refer to the book "Kinematic and Dynamic Simulation of Multibody Systems: The Real-Time Challenge" [56] for further details on the method

1.4 Main Contributions

1.4.1 Software Development

The group of researchers of Dr. Corina and Adrian Sandu have developed since 2010 a multibody dynamic software called MBSVT (Multibody Systems at Virginia Tech) capable of modeling any complex multibody system by providing the dynamic and kinematic solutions of the system. In addition, this software is built to provide the sensitivity of the solutions of the system with respect to parameters or initial conditions. The analysis can be performed with the direct sensitivity or the adjoint sensitivity analysis. To perform such analysis, MBSVT is linked to a numerical integrator package FATODE built in Dr. Adrian Sandu's laboratory. Both MBSVT and FATODE are are open source for research purpose and programmed in FORTRAN.

In more details, FATODE is an open source Fortran library [57] that contains the family of Runge-Kutta integrators for the forward, the tangent linear model (TLM), and the adjoint sensitivity for ODE and DAE systems. Four families of methods are implemented: "explicit Runge-Kutta for nonstiff problems and fully implicit Runge-Kutta, singly diagonally implicit Runge-Kutta, and Rosenbrock for stiff problems". The selection of the integrator depends of the type of model. As a rule of thumb, we run our simulation with two different integrators to ensure the convergence of the results.

The MBSVT packages is based of Cartesian coordinates located at the center of gravity of each body and of euler parameters for the body's orientation. Each body is linked together thanks to kinematic constraints. MBSVT contains a kinematic library of dot-1 constraint, revolute joint, spherical joint, translational constraint, distance constraint and coordinates driving constraints. The kinematic constrains are satisfied at each time step by using the penalty formulation, which is an ODE formulation that combines the equation of motion with the kinematic constraints.

In addition, the library implements external forces such as translational spring-damperactuator (TSDA), and different type of normal and tangential forces to simulate normal contact and friction, receptively.

Finally, MBSVT is associated with the optimization package L-BFGS-B, a gradient-based optimization algorithm, that uses the derivatives provided by the sensitivity analysis to determine the optimized trajectories and parameters values by minimizing the cost function related to the system performance.

New implementation on MBSVT projects New implementations in the MBSVT softwares allow the extraction of parameters, forces, and constraints information from text files. This enables the user to modify multibody model inputs without opening MBSVT. For complex systems, there is the possibility to extract this information directly from CAD files. A MATLAB code was created to generate an xml file from the CAD software and to transfer the necessary information to the MBSVT input text files. These newly added capabilities enhanced the MBSVT's applicability and reduced the model set-up phase. The following are examples of case studies which employed MBSVT:

- One of our main multibody model is the "Five-bars mechanism". It has been used to validate the mathematical framework of my research presented in this dissertation.
- The dynamic simulation of three different types of vehicles (Iltis, IVECO truck, and an agricultural tracked vehicle) have been accomplished (driving over a bump, handling maneuver, curving, etc. ...).

- In collaboration with the University of Technology of Compiegne, France, we are currently working on drone simulation and parameter sensitivity of such design based on the sensitivity methodology developed in this dissertation.

New capabilities of the MBSVT library. The MBSVT library, written in Fortran, gathers all the source code (20 files for a total of 6000 lines) that contains the mathematical relations needed to perform the dynamic analysis, the sensitivity analysis, and the optimization analysis for any multibody dynamic system. One of my contributions for MBSVT was to restructure the software to make it more robust and more efficient. (The earliest version suffered from its data structure and organization, which made any changes in the library difficult to process). Once restructured, the following new implementations or modifications were made:

- New implementations of all necessary mathematical relations presented in this dissertation, especially the jump sensitivity matrix that determines the forward state solution and the sensitivities after an event occurred.
- New implementations of all necessary kinematic functions with respect to time and parameters (the Jacobians, tensor, time derivative of the Jacobians, etc.) related to the the kinematic constrains (dot 1, revolute joint, spherical joint). These derivatives compose the required functions needed in the computation of the sensitivity analysis when the penalty formulation is used for modeling the system A.

- Validation codes to calculate the sensitivities based on the finite difference method. This method was used to benchmark the analytical sensitivities calculated with the mathematical framework contained in MBSVT library.

MBSVT / FATODE . My main contributions are the implementation of new features to incorporate FATODE into MBSVT. This work was done in collaboration with Mahesh Narayanamurthi:

- Features were implemented to have MBSVT library used for the forward dynamics, the TLM direct sensitivity, and the adjoint sensitivity FATODE integrators: RK, ERK, SDIRK, and ROS (a total of 12 integrators)
- A sensing pointer function was created to extract and print to external text files any values (states, force values, function evaluations, etc.) of interest at each time step.
- A new algorithm that implements event functions in the ERK FATODE integrator was implemented. The algorithm accounts for multiple events that enables exploring mechanisms with multiple contacts.

MATLAB symbolic A MATLAB symbolic library source code was implemented to efficiently calculate derivatives with respect to state variables, parameters and time of any kind of functions. This allows for example to determine the Jacobian of the constraints, the time derivative of the Jacobian and all other types of derivatives presented in A. The generated library has helped to explore the mathematical framework presented in this dissertation and validated it. The validation is presented through the stufy of the five-bar mechanism.

1.4.2 Theory Development

The main theoretical contributions are summarized in this section.

- Developed a unified methodology to compute the sensitivity of the state variables and any cost functions with respect to system parameters, for any systems governed by a second order ODE and rank 1 and 3 DAE systems. The theoretical framework is presented in a manner that facilitates its implementation and the analysis in a clear and efficient manner.
- Sensitivity analysis is performed by the Tangent Linear Model (forward mode) and adjoint model (backward mode). This dissertation shows a clear correlation between these two strategies in computing the sensitivity of the general cost function. Their correlation has not been presented in the literature, or not well identified. It is often said than the TLM is used for sensitivity analysis with few parameters, as the TLM sensitivity matrix extends its dimension according to the number of parameters. Similarly, the adjoint sensitivity analysis is used for sensitivity analysis with few cost functions, as the adjoint sensitivity matrix extends its dimension according to the number of cost functions. This dissertation clearly shows how these two approaches should be implemented and performed. The adjoint variables are abstractly difficult to conceptualize.

The presented correlation with the TLM variables helps better understand their utilities. This correlation supports reaching the main result presented in this dissertation, which is the sensitivity matrix of cost functions with respect to parameters for general HODE systems. Such a matrix is a key result for design analysis as it provides the parameters that affect the given cost functions the most. Such results could be applied to gradient based algorithms, control optimization, implicit time integration methods, deep learning, etc.

- This study shows that any mechanical systems governed by ODE and DAE is dependent on four types of variables: the time, the position, the velocity, and the parameters. This fact may be simple, but their correlation is actually not straight forward. Visual representations are given in this dissertation that help the reader better understand this correlation. The evolution of the four variables vary in the time-space domain due to the evaluation of the governing functions (ODE or DAE). This is why any derivatives of these functions could only be with respect to these variables. It has been shown that the derivative of a cost function with respect to the acceleration variable can be simplified to the derivative with respect to position and velocity. Such simplification is a key result in this dissertation, as it allows writing many complex formulations in a simple and easy manner.
- This dissertation contributes to the jumping conditions for the TLM and the adjoint sensitivity matrix approaches. The mathematical framework computes the jump sensitivity matrix of the direct sensitivities that jumps the sensitivity matrix from its value

right before an event to its new values right after the event. Such jumps happen because of the piece-wise trajectories of the forward solution of a system. The main idea is then to obtain the transpose of the jump sensitivity matrix to compute the jump conditions for the adjoint sensitivities.

1.5 Outline of Dissertation

The dissertation is organized as follows: A description of the direct sensitivity approach for smooth and hybrid, non-constrained and constrained mechanical systems is introduced in Chapter 2. The extension of the previous methodology and approach adjoint sensitivty analysis is presented in Chapter 3. Presented at the end of Chapter 2 and 3, a study of the five-bar mechanism is presented which aims to validate the mathematical framework developed in these chapters. Main contribution and Conclusions are drawn in Chapter 4, respectively .

Chapter 2

Modeling And Direct Sensitivity Analysis Methodology

2.1 Direct sensitivity analysis for smooth ODE systems

We start the discussion with a review of direct sensitivity analysis for dynamical systems governed by smooth ODEs.

2.1.1 Smooth ODE systems dynamics

In this study we consider second order systems of ordinary differential equations of the form:

$$\mathsf{M}\left(t, q, \rho\right) \cdot \ddot{q} = \mathsf{F}\left(t, q, \dot{q}, \rho\right), \quad t_0 \le t \le t_F, \quad q(t_0) = q_0(\rho), \quad \dot{q}(t_0) = \dot{q}_0(\rho), \tag{2.1}$$

or equivalently:

$$\ddot{q} = \mathsf{M}^{-1}(t, q, \rho) \cdot \mathsf{F}(t, q, \dot{q}, \rho) =: f^{\text{eom}}(t, q, \dot{q}, \rho), \tag{2.2}$$

that arise from the description of the dynamics of mechanical systems. In (2.2) $t \in \mathbb{R}$ is time, $q \in \mathbb{R}^n$ is the generalized position vector and $\dot{q} \in \mathbb{R}^n$ is the generalized velocity vector, n is the dimension of generalized coordinates, and $\rho \in \mathbb{R}^p$ is the vector of system parameters, where p is the number of parameters. The dot notation ($\dot{\Box}$ or $\ddot{\Box}$) indicates the total (first or second order) derivative of a function or variable with respect to time. Subscripts indicate partial derivative with respect to a quantity, unless stated otherwise. The mass matrix $\mathsf{M} : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^{n \times n}$ is assumed to be smooth with respect to all its arguments, invertible, and with an inverse M^{-1} that is also smooth with respect to all arguments. The right-hand side function $\mathsf{F} : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^n$ represents external and internal generalized forces and is assumed to be smooth with respect to all its arguments.

The state trajectories are obtained by integrating the equations of motion (2.2), which depend on the system parameters ρ. Consequently, the state trajectories (the solutions of the equations of motion) depend implicitly on time and on the parameters, $q = q(t, \rho)$ and $\dot{q} = \dot{q}(t, \rho)$. The state trajectories also depend implicitly on the initial conditions of (2.2). For clarity we denote the velocity state variables by $v = \dot{q} \in \mathbb{R}^n$.

Sensitivity analysis computes derivatives of the solutions of (2.2) with respect to the system parameters:

$$Q(t,\rho) := D_\rho q(t) := \frac{dq}{d\rho}(t,\rho) \in \mathbb{R}^{n\times p}, \quad V(t,\rho) := D_\rho v(t) = \frac{dv}{d\rho}(t,\rho) \equiv \frac{d\dot{q}}{d\rho}(t,\rho) = \dot{Q}(t,\rho) \in \mathbb{R}^{n\times p}. \tag{2.3}$$

The second order ODE (2.2) can be transformed into a first order reduced system as follows. With the velocity state variables $v := \dot{q} \in \mathbb{R}^n$ the system (2.2) can be written in the form:

$$\begin{bmatrix} \mathsf{I} & \mathsf{0} \\ \mathsf{0} & \mathsf{M}(t,q,\rho) \end{bmatrix} \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ \mathsf{F}(t,q,v,\rho) \end{bmatrix} \quad \Leftrightarrow \quad \begin{bmatrix} \dot{q} \\ \dot{v} \end{bmatrix} = \begin{bmatrix} v \\ f^{\text{eom}}\,(t,q,v,\rho) \end{bmatrix}, \qquad \begin{bmatrix} q(t_0) \\ v(t_0) \end{bmatrix} = \begin{bmatrix} q_0(\rho) \\ v_0(\rho) \end{bmatrix}. \tag{2.4}$$

Definition 2.1.1 (Cost function)**.** Consider a smooth 'trajectory cost function' $g : \mathbb{R}^{1+3n+p} \to \mathbb{R}$ and a smooth 'terminal cost function' $w : \mathbb{R} \times \mathbb{R}^{1+2n+p} \to \mathbb{R}$. A general cost function is defined as the sum of the costs along the trajectory plus the cost at the terminal point of the solution:

$$\psi = \int_{t_0}^{t_F} g\,(\,t,\, q,\, v,\, \dot{v},\, \rho\,)\ dt + w\big(t_F, q(t_F,\rho), v(t_F,\rho), \rho\big). \tag{2.5}$$

Remark (Accelerations in the cost function). Note that the trajectory cost function (2.5) includes accelerations via $\dot{v}$. Accelerations are not independent variables and they can be resolved in terms of positions and velocities:

$$g\,(\,t,\, q,\, v,\, \dot{v},\, \rho\,) = g\big(\,t,\, q,\, v,\, f^{\text{eom}}(t,q,v,\rho),\, \rho\,\big) = \tilde{g}\big(\,t,\, q,\, v,\, \rho\,\big). \tag{2.6}$$

We prefer to keep accelerations as an explicit argument in the cost function (2.5) in order to give additional flexibility in practical applications. However, we will need to resolve the sensitivities of acceleration in terms of other sensitivities in subsequent calculations.

To further simplify the notation we define the 'quadrature' variable $z(t) \in \mathbb{R}$ as follows:

$$\begin{aligned} &z(t,\rho) := \int_{t_0}^{t} \tilde{g}\big(t, q(t,\rho), v(t,\rho), \rho\big)\, dt \quad \Leftrightarrow \\ &\dot{z}(t,\rho) = g\,(\,t,\, q,\, v,\, \dot{v},\, \rho\,) = \tilde{g}\big(t, q(t,\rho), v(t,\rho), \rho\big), \quad t_0 \le t \le t_F, \quad z(t_0,\rho) = 0. \end{aligned} \tag{2.7}$$

The cost function (2.5) reads:

$$\psi = z(t_F,\rho) + w\big(t_F, q(t_F,\rho), v(t_F,\rho), \rho\big). \tag{2.8}$$

Definition 2.1.2 (The canonical ODE system)**.** The canonical system is obtained by combining the first order ODE dynamics (2.4) with equation (2.7) for the 'quadrature' variable':

$$\begin{aligned} x(t) \;\; &:= \begin{bmatrix} q(t) \\ v(t) \\ z(t) \end{bmatrix} \in \mathbb{R}^{2n+1}; \qquad \dot{x} = \begin{bmatrix} \dot{v} \\ f^{\text{eom}}\big(t, q(t,\rho), v(t,\rho), \rho\big) \\ \tilde{g}(\,t,\, q,\, v,\, \rho\,) \end{bmatrix} = F(t,x,\rho), \\ & t_0 \le t \le t_F, \quad x(t_0,\rho) = \begin{bmatrix} q_0(\rho)^{\mathrm{T}} & v_0(\rho)^{\mathrm{T}} & 0 \end{bmatrix}^{\mathrm{T}}. \end{aligned} \tag{2.9a}$$

The canonical cost function (2.8) is purely a terminal cost function:

$$\psi = z(t_F, \rho) + w\big(t_F, q(t_F, \rho), v(t_F, \rho), \rho\big) = W\big(x(t_F, \rho), \rho\big). \tag{2.9b}$$

2.1.2 Direct sensitivity approach for smooth ODE systems

Definition 2.1.3 (The sensitivity analysis problem)**.** Our goal in this work is to perform a sensitivity analysis of the cost function, i.e., to compute the total derivative of the cost function (2.5) with respect to model parameters ρ:

$$D_\rho \psi = \frac{d\,\psi}{d\,\rho} \in \mathbb{R}^{1\times p}. \tag{2.10}$$

Note that the cost function (2.5) depends on the system parameters ρ directly (through the direct dependency of g and w on ρ) as well as indirectly (through the dependency of q and v on ρ). The sensitivity (2.10) needs to account for all the direct and the indirect dependencies.

Remark (The direct sensitivity analysis approach). In order to compute the sensitivity (2.10) we take a variational calculus approach [58, 27, 2]. Infinitesimal changes in parameters

$$\rho \to \rho + \delta\rho \in \mathbb{R}^p, \tag{2.11}$$

lead to a total change in the cost function as follows:

$$\psi \rightarrow \psi + \delta\psi, \quad \delta\psi = \sum_{i=1}^{p} \frac{d\psi}{d\rho_i} \cdot \delta\rho_i = D_\rho\psi \cdot \delta\rho. \tag{2.12}$$

The direct sensitivity analysis computes each element $(D_\rho\psi)_i = \partial\psi/\partial\rho_i$ of the derivative (2.10) by accounting for changes in the cost function that result from changing each individual parameter $\delta\rho_i$, $i = 1 \ldots p$.

2.1.3 Direct sensitivity analysis with respect to system parameters solved analytically

Definition 2.1.4 (The tangent linear model (TLM))**.** Consider the 'position sensitivity' matrix $Q(t,\rho)$ and the 'velocity sensitivity' matrix $V(t,\rho)$ defined in (2.3):

$$\begin{aligned} Q_i(t,\rho) &:= \tfrac{d\,q(t,\rho)}{d\,\rho_i} \in \mathbb{R}^n, \quad i = 1,\ldots,p; \quad Q(t,\rho) := \begin{bmatrix} Q_1(t,\rho) \cdots Q_p(t,\rho) \end{bmatrix} \in \mathbb{R}^{n\times p}, && \text{(2.13a)} \\ V_i(t,\rho) &:= \tfrac{d\,v(t,\rho)}{d\,\rho_i} \in \mathbb{R}^n, \quad i = 1,\ldots,p; \quad V(t,\rho) := \begin{bmatrix} V_1(t,\rho) \cdots V_p(t,\rho) \end{bmatrix} \in \mathbb{R}^{n\times p}. && \text{(2.13b)} \end{aligned}$$

These sensitivities evolve in time according to the *tangent linear model* (TLM) equations [58, 27, 2], obtained by differentiating the equations of motion (2.2) with respect to the parameters:

$$\begin{cases} \dot{Q}_i &= \dfrac{d\dot{q}}{d\rho_i} = \dfrac{dv}{d\rho_i} = V_i, \\ \dot{V}_i &= \dfrac{d\dot{v}}{d\rho_i} = f^{\text{eom}}_q\,(t,q,v,\rho)\cdot\dfrac{dq}{d\rho_i} + f^{\text{eom}}_v\,(t,q,v,\rho)\cdot\dfrac{dv}{d\rho_i} + f^{\text{eom}}_{\rho_i}\,(t,q,v,\rho) \\ &= f^{\text{eom}}_q\,(t,q,v,\rho)\cdot Q_i + f^{\text{eom}}_v\,(t,q,v,\rho)\cdot V_i + f^{\text{eom}}_{\rho_i}\,(t,q,v,\rho)\,, \\ & \qquad i = 1,\ldots,p, \quad t_0 \le t \le t_F, \end{cases} \tag{2.14a}$$

with the initial conditions

$$Q_i(t_0,\rho) = \frac{dq_0}{d\rho_i}, \quad V_i(t_0,\rho) = \frac{dv_0}{d\rho_i}, \quad i = 1,\ldots,p. \tag{2.14b}$$

The expressions f^{eom}_q, f^{eom}_v, and $f^{\text{eom}}_{\rho_i}$ denote the partial derivatives of f^{eom} with respect to the subscripted variables.

Remark. The partial derivatives $\partial f^{\text{eom}}/\partial\zeta$ are obtained by differentiating (2.2) with respect to $\zeta \in \{q, v, \rho\}$:

$$\frac{\partial f^{\text{eom}}}{\partial\zeta} = \frac{\partial(\mathsf{M}^{-1}\,\mathsf{F})}{\partial\zeta} = -\mathsf{M}^{-1}\mathsf{M}_\zeta\mathsf{M}^{-1}\,\mathsf{F} + \mathsf{M}^{-1}\,\mathsf{F}_\zeta = \mathsf{M}^{-1}\,\left(\mathsf{F}_\zeta - \mathsf{M}_\zeta\, f^{\text{eom}}\right) = \mathsf{M}^{-1}\,\left(\mathsf{F}_\zeta - \mathsf{M}_\zeta\,\dot{v}\right). \tag{2.15}$$

Definition 2.1.5 (The quadrature sensitivity)**.** Similarly, let the 'quadrature sensitivity' vector $Z(t,\rho)$ be the Jacobian of the 'quadrature' variable $z(t,\rho)$ (2.7) with respect to the parameters ρ:

$$Z_i(t,\rho) := \frac{\partial z(t,\rho)}{\partial \rho_i}, \quad i = 1,\dots,p; \quad Z(t,\rho) := \nabla_\rho z(t,\rho) = \Big[Z_1(t,\rho) \cdots Z_p(t,\rho) \Big] \in \mathbb{R}^{1\times p}. \tag{2.16}$$

The time evolution equations of the quadrature sensitivities are given by the TLM obtained by differentiating (2.7) with respect to the parameters:

$$\begin{aligned} \dot{Z}_i = \frac{d\, g\,(\,t,\, q,\, v,\, \dot{v},\, \rho\,)}{d\,\rho_i} &= g_q \cdot Q_i + g_v \cdot V_i + g_{\dot{v}} \cdot \dot{V}_i + g_{\rho_i} \\ &= \big(g_q + g_{\dot{v}}\, f_q^{\text{eom}}\big) \cdot Q_i + \big(g_v + g_{\dot{v}}\, f_v^{\text{eom}}\big) \cdot V_i + g_{\rho_i} + g_{\dot{v}} \cdot f_{\rho_i}^{\text{eom}}, \\ &\quad t_0 \le t \le t_F, \quad Z_i(t_0,\rho) = 0, \quad i = 1,\dots,p. \end{aligned} \tag{2.17}$$

Definition 2.1.6 (Canonical sensitivity ODE)**.** The solutions given by (2.9a), the TLM given by (2.14), and the sensitivity quadrature equations (2.62) need to be solved together forward in time, leading to the canonical sensitivity ODE that computes the derivatives of the cost function with respect to the system parameters ρ for smooth systems:

$$\begin{bmatrix} \dot{q} \\ \dot{v} \\ \dot{z} \\ \big[\dot{Q}_i\big]_{i=1,\dots,p} \\ \big[\dot{V}_i\big]_{i=1,\dots,p} \\ \big[\dot{Z}_i\big]_{i=1,\dots,p} \end{bmatrix} = \begin{bmatrix} v \\ f^{\text{eom}} \\ \tilde{g} \\ \big[V_i\big]_{i=1,\dots,p} \\ \big[f_q^{\text{eom}} Q_i + f_v^{\text{eom}} V_i + f_{\rho_i}^{\text{eom}}\big]_{i=1,\dots,p} \\ \big[\big(g_q + g_{\dot{v}}\, f_q^{\text{eom}}\big) \cdot Q_i + \big(g_v + g_{\dot{v}}\, f_v^{\text{eom}}\big) \cdot V_i + g_{\rho_i} + g_{\dot{v}} \cdot f_{\rho_i}^{\text{eom}}\big]_{i=1,\dots,p} \end{bmatrix}, \tag{2.18}$$

where the state vector of the canonical sensitivity ODE is :

$$X = \left[\, q^{\mathrm{T}},\, v^{\mathrm{T}},\, z,\; Q_1^{\mathrm{T}}, \ldots, Q_p^{\mathrm{T}},\, V_1^{\mathrm{T}}, \ldots, V_p^{\mathrm{T}},\, Z_1, \ldots, Z_p \right]^{\mathrm{T}} \in \mathbb{R}^{(n+1)(p+1)}. \tag{2.19}$$

Remark (The sensitivities of the cost function). Once the quadrature sensitivities (2.17) have been calculated, the sensitivities of the cost function with respect to each parameter are computed as follows:

$$\begin{aligned}\frac{d\,\psi}{d\,\rho_i} &= Z_i(t_F) + w_q\big(\,t_F,\, q(t_F,\rho),\, v(t_F,\rho),\, \rho\,\big)\cdot Q_i(t_F,\rho) + w_v\big(\,t_F,\, q(t_F,\rho),\, v(t_F,\rho),\, \rho\,\big)\cdot V_i(t_F,\rho)\\ &\quad + w_{\rho_i}\big(\,t_F,\, q(t_F,\rho),\, v(t_F,\rho),\, \rho\,\big), \qquad i = 1, \ldots, p.\end{aligned} \tag{2.20}$$

2.1.4 Direct sensitivity analysis with respect to system parameters solved with the complex finite difference method

An accurate numerical method for sensitivity analysis of a smooth ODE system with respect to the system parameters ρ is the complex finite difference method [58, 27, 2]. Add a small *complex* perturbation to one parameter:

$$\tilde{\rho}_j = \begin{cases} \rho_j & \text{for } \; j \neq \ell, \\ \rho_\ell + \mathfrak{i}\,\Delta\rho & \text{for } \; j = \ell, \end{cases} \qquad j = 1, \ldots, p, \tag{2.21}$$

and solve the canonical ODE system (2.9a) for this perturbed values of the parameters to obtain:

$$q(t,\tilde{\rho}), \quad v(t,\tilde{\rho}), \quad z(t,\tilde{\rho}), \quad \psi(\tilde{\rho}) = z(t_F,\tilde{\rho}) + w\big(\, q(t_F,\tilde{\rho}),\, v(t_F,\tilde{\rho}),\, \tilde{\rho}\,\big). \tag{2.22}$$

The sensitivities are approximated numerically by the imaginary parts of the state variables:

$$Q_\ell(t,\rho) \approx -\frac{\mathrm{imag}\big(q(t,\tilde{\rho})\big)}{\|\Delta\rho\|}, \quad V_\ell(t,\rho) \approx -\frac{\mathrm{imag}\big(v(t,\tilde{\rho})\big)}{\|\Delta\rho\|}, \quad \frac{d\,\psi}{d\,\rho_\ell} \approx -\frac{\mathrm{imag}\big(\psi(\tilde{\rho})\big)}{\|\Delta\rho\|}. \tag{2.23}$$

We next discuss an approach to sensitivity analysis that accounts for discontinuities in the state variables.

2.2 Direct sensitivity analysis for hybrid ODE system

2.2.1 Hybrid ODE system

Definition 2.2.1 (Hybrid dynamics)**.** A hybrid mechanical system is a piecewise-in-time continuous dynamic ODE described by (2.2) that exhibits discontinuous dynamic behavior in the generalized velocity state vector at a finite number of time moments (no zeno phenomenon [59]). Each such moment is a 'time of event' t_{eve} and corresponds to a triggering event described by the equation:

$$r\big(q|_{t_{\text{eve}}}\big) = 0, \tag{2.24}$$

where $r : \mathbb{R}^n \to \mathbb{R}$ is a smooth 'event function'.

Remark. In the context of this study, we assume that there are no grazing phenomenon where the system trajectory would make tangential contact with an the event triggering hypersurface [60, 61, 59].

Definition 2.2.2 (Characterization of an event)**.** For hybrid systems variables can change values during the event. For this reason we distinguish between the value of a variable right before the event $\boldsymbol{x}|^-_{t_{\text{eve}}}$, and its value right after the event $\boldsymbol{x}|^-_{t_{\text{eve}}}$:

$$\boldsymbol{x}|^-_{t_{\text{eve}}} := \lim_{\varepsilon>0,\ \varepsilon\to 0} \boldsymbol{x}(t_{\text{eve}} - \varepsilon), \quad \boldsymbol{x}|^+_{t_{\text{eve}}} := \lim_{\varepsilon>0,\ \varepsilon\to 0} \boldsymbol{x}(t_{\text{eve}} + \varepsilon). \tag{2.25}$$

The limits exist since the evolution of the system is smooth in time both before and after the event.

We consider an event happening at time t_{eve} that applies a finite energy impulse force to the system. Such an impulse force does not change the generalized position state variables, and therefore:

$$q|^+_{t_{\text{eve}}} = q|^-_{t_{\text{eve}}} = q|_{t_{\text{eve}}}. \tag{2.26}$$

However, the finite energy event can abruptly change the generalized velocity state vector $\dot{q}$ from its value $v|^-_{t_{\text{eve}}}$ right before the event to a new value $v|^+_{t_{\text{eve}}}$ right after the event. The 'jump function' at the time of event t_{eve} characterizes the change in the generalized velocity during the event:

$$v|_{t_{\text{eve}}}^{+} = h\Big(t_{\text{eve}},\, q|_{t_{\text{eve}}},\, v|_{t_{\text{eve}}}^{-},\, \rho\Big) \quad \Leftrightarrow \quad \dot{q}|_{t_{\text{eve}}}^{+} = h\Big(t_{\text{eve}},\, q|_{t_{\text{eve}}},\, \dot{q}|_{t_{\text{eve}}}^{-},\, \rho\Big). \tag{2.27}$$

Remark (Multiple events). In many cases the change can be triggered by one of multiple events. Each individual event is described by the event function $r_\ell : \mathbb{R}^n \to \mathbb{R}$, $\ell = 1, \ldots, e$. The detection of the next event, which can be one of the possible e options, is described by:

$$r_1\big(q|_{t_{\text{eve}}}\big) \cdot r_2\big(q|_{t_{\text{eve}}}\big) \ \ldots \ r_e\big(q|_{t_{\text{eve}}}\big) = 0, \tag{2.28}$$

and if event ℓ takes place then $r_\ell = 0$ and the corresponding jump is:

$$v|_{t_{\text{eve}}}^{+} = h_\ell\Big(q|_{t_{\text{eve}}},\, v|_{t_{\text{eve}}}^{-}\Big). \tag{2.29}$$

Remark (Numerical implementation of events). Numerical solutions of hybrid systems use an event detection mechanism. The event function (2.24) is implemented in the numerical time solver such that the integrator is stopped at the solution of (2.24). The jump function (2.27) is implemented as a callback function that is executed after the event is detected. The numerical integration resumes with new initial conditions after the jump.

Definition 2.2.3 (Twin perturbed systems)**.** Consider two versions of the system (2.2) with identical dynamics and initial conditions, but with different parameters values ρ_1 and

ρ_2, respectively. Without loss of generality in this proof we consider the scalar parameter case $p = 1$; the general equation (2.33) can be proven element by element by considering sensitivities with respect to individual parameters. The two parameters are infinitesimally small perturbations $\delta\rho$ of the reference parameter value ρ:

$$\rho_1 = \rho - \frac{\delta\rho}{2}; \qquad \rho_2 = \rho + \frac{\delta\rho}{2}. \tag{2.30}$$

We denote by $q_1(t) = q(t, \rho_1)$, $v_1(t) = v(t, \rho_1)$, and $z_1(t) = z(t, \rho_1)$ the position and velocity states, and the quadrature variable of the first system, respectively. We denote by $q_2(t) = q(t, \rho_2)$, $v_2(t) = v(t, \rho_2)$, and $z_2(t) = z(t, \rho_2)$ the position and velocity states, and the quadrature variable of the second system, respectively.

Assume that the sign of the perturbation $\delta\rho$ is such that $\tau_2 > t_{\text{eve}} > \tau_1$, and denote $\delta\tau = \tau_2 - \tau_1$. Since $\delta\rho$ is infinitesimally small, so is $\delta\tau$. The trajectories of the positions $q(t)$, $q_1(t)$, and $q_2(t)$, as well as the trajectories of the velocities $v(t)$, $v_1(t)$, and $v_2(t)$, are schematically illustrated in Fig. 2.1 and Fig. 2.2, respectively. As shown in Fig. 2.1 the first system meets the event described by the function (2.24) at the time of event $t_{\text{eve}}(\rho_1) = \tau_1$, when its position state is $q_1|_{\tau_1}$. The second system meets the event at time $t_{\text{eve}}(\rho_2) = \tau_2$, when its position state is $q_2|_{\tau_2}$. Note that in the limit of vanishing $\delta\rho$ we have:

$$\begin{aligned} \delta\rho \to 0 \quad \Rightarrow \quad & v_1|_{\tau_1}^{-} \to v|_{t_{\text{eve}}}^{-}, \quad v_1|_{\tau_2} \to v|_{t_{\text{eve}}}^{+}, \quad v_1|_{\tau_1}^{+} \to v|_{t_{\text{eve}}}^{+}; \\ & v_2|_{\tau_1} \to v|_{t_{\text{eve}}}^{-}, \quad v_2|_{\tau_2}^{-} \to v|_{t_{\text{eve}}}^{-}, \quad v_2|_{\tau_2}^{+} \to v|_{t_{\text{eve}}}^{+}. \end{aligned} \tag{2.31}$$

Let $Q|^+_{t_{\text{eve}}}, Q|^-_{t_{\text{eve}}} \in \mathbb{R}^{n\times p}$ be the sensitivities of the generalized positions (2.13a) right before and right after the event, respectively. Let $V|^+_{t_{\text{eve}}}, V|^-_{t_{\text{eve}}} \in \mathbb{R}^{n\times p}$ be the sensitivities of the generalized velocities (2.13b) right before and right after the event, respectively. Our methodology to find these sensitivities is to first evaluate the states $q_1(t), v_1(t)$ and $q_2(t), v_2(t)$ of each of the twin perturbed systems at both τ_1 and τ_2. The sensitivities are obtained from their definition by taking differences of states of the two systems, dividing them by the perturbation in parameters, and taking the limits, for example:

$$Q_i|^-_{t_{\text{eve}}} = \lim_{\delta\rho_i \to 0} \frac{q_2|_{\tau_1} - q_1|_{\tau_1}}{\delta\rho_i}, \quad V_i|^+_{t_{\text{eve}}} = \lim_{\delta\rho_i \to 0} \frac{v_2|^+_{\tau_2} - v_1|_{\tau_2}}{\delta\rho_i}, \quad i = 1, \ldots, p. \tag{2.32}$$

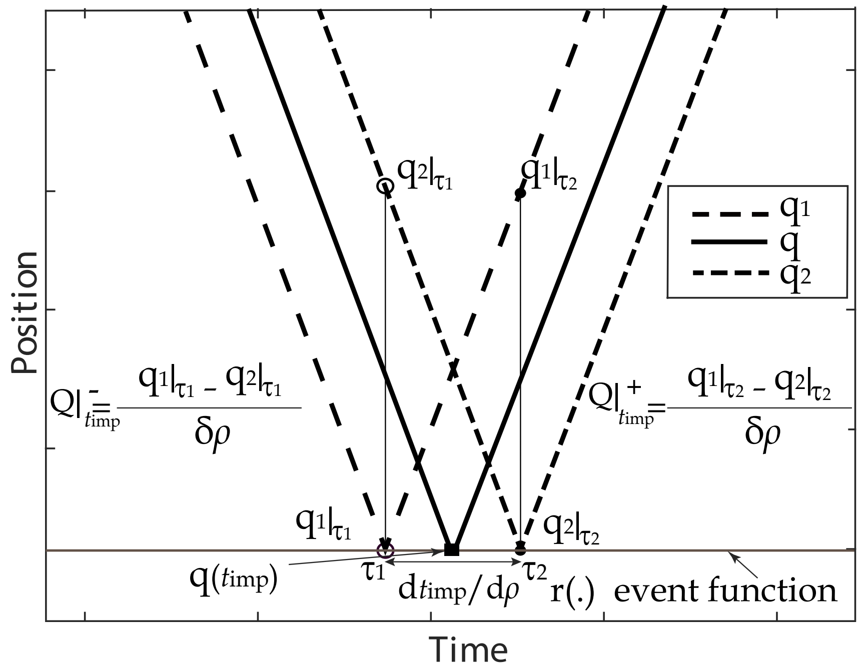


Figure 2.1: Schematic visualization of the jump in the sensitivity of the position.

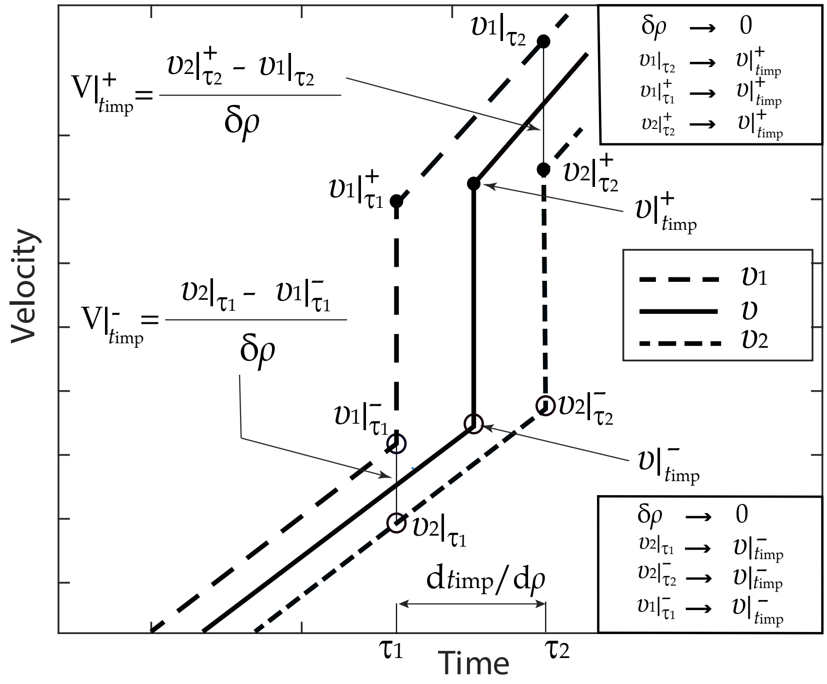


Figure 2.2: Schematic visualization of the jump in the sensitivity of the velocity.

2.2.2 The sensitivity of the time of event with respect to the system parameters

Theorem 1 (Sensitivity of the time of event [62, 43, 41, 35, 34, 38])**.** *Let* $r(\cdot) \in \mathbb{R}$ *be the scalar event function defined by* (2.24)*, and* $dr/dq \in \mathbb{R}^{1\times n}$ *be its Jacobian. The sensitivity of the time of event with respect to the system parameters is:*

$$\frac{dt_{\mathrm{eve}}}{d\rho} = -\frac{\dfrac{dr}{dq}\left(q|_{t_{\mathrm{eve}}}\right) \cdot Q|^-_{t_{\mathrm{eve}}}}{\dfrac{dr}{dq}\left(q|_{t_{\mathrm{eve}}}\right) \cdot v|^-_{t_{\mathrm{eve}}}} \in \mathbb{R}^{1\times p}. \tag{2.33}$$

Proof. *The time at which the event function becomes zero is indirectly dependent on the system parameters* ρ*. We evaluate the derivative of equation* (2.24) *with respect to the system parameters:*

$$0 = r\,\left(q(t_{\text{eve}},\rho)\right) \quad \Rightarrow \quad 0 = \frac{dr}{d\rho} = \frac{dr}{dq}\left(\frac{dq}{d\rho} + \dot{q}\,\frac{dt_{\text{eve}}}{d\rho}\right). \tag{2.34}$$

Rearrange the terms in (2.34) *to obtain* (2.33). ☐

Remark. The sensitivity of the time of event with respect to the system parameters exists only for situations that do not involve grazing where $\frac{dr}{dq} = 0$ for such case.

2.2.3 The jump in the sensitivity of the position state vector due to the event

This section provides the jumps in the sensitivities of the position state vector $q(t)$ at the time of event [62, 43, 41, 35, 34, 38]. Due to the nonzero inertia, the position state variable is continuous in time (2.26). However, its sensitivity can be discontinuous at the time of event, as established next.

Theorem 2 (Jump in position sensitivity [62, 43, 41, 36])**.** *Let* $v|_{t_{\text{eve}}}^{+}, v|_{t_{\text{eve}}}^{-} \in \mathbb{R}^n$ *be the generalized velocity state vectors after and before the event, respectively; the corresponding velocity jump function was introduced in* (2.27)*. Let* $Q|_{t_{\text{eve}}}^{+}$ *and* $Q|_{t_{\text{eve}}}^{-} \in \mathbb{R}^{n\times p}$ *be the sensitivities of the generalized position state vectors after and before the event, respectively. The* *jump equation of the sensitivities of the generalized position state vector is:*

$$Q|_{t_{\mathrm{eve}}}^{+} = Q|_{t_{\mathrm{eve}}}^{-} - \left(v|_{t_{\mathrm{eve}}}^{+} - v|_{t_{\mathrm{eve}}}^{-}\right) \cdot \frac{dt_{\mathrm{eve}}}{d\rho}. \tag{2.35}$$

Proof. *Consider the twin perturbed systems from Definition 2.2.3. The evolution of positions is illustrated in Fig. 2.1, where the two different dashed line trajectories represent the position variables of the two perturbed systems. The jump in the velocity state variables occurs at time* τ_1 *only for the first system. The position variables at time* τ_2 *for both systems are:*

$$\begin{aligned} q_1|_{\tau_2} &= q_1|_{\tau_1} + h\big(v_1|_{\tau_1}^{-}\big)\, \delta\tau, \\ q_2|_{\tau_2} &= q_2|_{\tau_1} + v_2|_{\tau_1}\, \delta\tau. \end{aligned} \tag{2.36}$$

Subtract the two equations and scale by the perturbation in the parameters:

$$\frac{q_2|_{\tau_2} - q_1|_{\tau_2}}{\delta\rho} = -\left(v_1|_{\tau_1}^{+} - v_2|_{\tau_1}\right) \frac{\delta\tau}{\delta\rho} + \frac{q_2|_{\tau_1} - q_1|_{\tau_1}}{\delta\rho}. \tag{2.37}$$

Using (2.31) *and taking the limit* $\delta\rho \to 0$ *in* (2.37) *we obtain* (2.35)*. The trajectory state differences are illustrated by the vertical lines in Fig. 2.1.*

2.2.4 The jump in the sensitivity of the velocity state vector due to the event

This section provides the jumps in the sensitivities of the velocity state vector $v(t)$ at the time of event [41, 35, 34, 38] corresponding to the jump function (2.27).

Theorem 3 (Jump in velocity sensitivity.). *[41, 35, 34, 38] Let* $V|^{+}_{t_{\rm eve}}, V|^{-}_{t_{\rm eve}} \in \mathbb{R}^{n\times p}$ *be the sensitivities of the generalized position state vectors after and before the event, respectively. Let* $v|^{+}_{t_{\rm eve}}$ *and* $v|^{-}_{t_{\rm eve}} \in \mathbb{R}^{n}$ *be the velocity state vectors after and before the event affected by the jump function* (2.27) *, respectively. Let* $\ddot{q}|^{+}_{t_{\rm eve}}$ *and* $\ddot{q}|^{-}_{t_{\rm eve}} \in \mathbb{R}^{n}$ *be the generalized acceleration state vectors after and before the event, respectively. The jump equation of the sensitivities of the generalized velocity state vector is:*

$$\begin{aligned} V|^{+}_{t_{\rm eve}} &= h_q|^{-}_{t_{\rm eve}} \cdot Q|^{-}_{t_{\rm eve}} + h_v|^{-}_{t_{\rm eve}} \cdot V|^{-}_{t_{\rm eve}} \\ &\quad + \left(h_q|^{-}_{t_{\rm eve}} \cdot v|^{-}_{t_{\rm eve}} - \ddot{q}|^{+}_{t_{\rm eve}} + h_v|^{-}_{t_{\rm eve}} \cdot \ddot{q}|^{-}_{t_{\rm eve}} + h_t|^{-}_{t_{\rm eve}}\right) \cdot \frac{dt_{\rm eve}}{d\rho} + h_\rho|^{-}_{t_{\rm eve}}, \end{aligned} \tag{2.38}$$

where the Jacobians of the jump function are:

$$\begin{aligned} h_t|^{-}_{t_{\rm eve}} &:= \frac{\partial h}{\partial t}\left(t_{\rm eve}, q|_{t_{\rm eve}}, v|^{-}_{t_{\rm eve}}, \rho\right) \in \mathbb{R}^{f}, & h_q|^{-}_{t_{\rm eve}} &:= \frac{\partial h}{\partial q}\left(t_{\rm eve}, q|_{t_{\rm eve}}, v|^{-}_{t_{\rm eve}}, \rho\right) \in \mathbb{R}^{f\times n}, \\ h_v|^{-}_{t_{\rm eve}} &:= \frac{\partial h}{\partial v}\left(t_{\rm eve}, q|_{t_{\rm eve}}, v|^{-}_{t_{\rm eve}}, \rho\right) \in \mathbb{R}^{f\times f}, & h_\rho|^{-}_{t_{\rm eve}} &:= \frac{\partial h}{\partial \rho}\left(t_{\rm eve}, q|_{t_{\rm eve}}, v|^{-}_{t_{\rm eve}}, \rho\right) \in \mathbb{R}^{f\times p}. \end{aligned} \tag{2.39}$$

Proof. *We consider again the twin perturbed systems from Definition 2.2.3. The jumps in* *velocities are illustrated in Fig. 2.2. The velocities for each system are determined as follows:*

$$\begin{aligned}
v_1|_{\tau_2} &= v_1|^{+}_{\tau_1} + f^{\text{eom}}\Big(\tau_1,\, q_1|_{\tau_1},\, v_1|^{+}_{\tau_1},\, \rho_1\Big)\,\delta\tau, \\
&= h\big(\tau_1,\, q_1|_{\tau_1},\, v_1|^{-}_{\tau_1},\, \rho_1\big) + f^{\text{eom}}\Big(\tau_1,\, q_1|_{\tau_1},\, h\Big(\tau_1,\, q_1|_{\tau_1},\, v_1|^{-}_{\tau_1},\, \rho_1\Big),\, \rho_1\Big)\,\delta\tau, \\
v_2|^{+}_{\tau_2} &= h\ \big(\tau_2,\, q_2|_{\tau_2},\, v_2|^{-}_{\tau_2},\, \rho_2\ \big) \\
&= h\ \Big(\tau_2,\, q_2|_{\tau_1} + v_2|_{\tau_1}\ \delta\tau,\ v_2|_{\tau_1} + f^{\text{eom}}\Big(\tau_1,\, q_2|_{\tau_1},\, v_2|_{\tau_1},\, \rho_2\Big)\,\delta\tau,\, \rho_2\ \Big) \\
&\approx h\big(\tau_2,\, q_2|_{\tau_1}, v_2|_{\tau_1},\, \rho_2\ \big)\ +\ \frac{dh}{dq}\big(q_2|_{\tau_1}, v_2|_{\tau_1}\big)\cdot v_2|_{\tau_1}\ \delta\tau \\
&+ \frac{dh}{dv}\big(q_2|_{\tau_1}, v_2|_{\tau_1}\big)\cdot f^{\text{eom}}\Big(\tau_1,\, q_2|_{\tau_1},\, v_2|_{\tau_1},\, \rho_2\Big)\,\delta\tau,
\end{aligned} \tag{2.40}$$

where f^{eom} is the instantaneous acceleration of the system from (2.2). The last relation represents a linearization (first order Taylor expansion) that is infinitely accurate since $\delta\tau$ is infinitesimally small. The scaled difference between the velocity state vectors at the time *of event is :*

$$
\begin{aligned}
& \frac{v_2|^+_{\tau_2} - v_1|_{\tau_2}}{\delta\rho} \\
\approx \quad & \frac{h\big(\,\tau_2,\, q_2|_{\tau_1}, v_2|_{\tau_1},\, \rho_2\,\big) - h\big(\,\tau_1,\, q_1|_{\tau_1}, v_1|^-_{\tau_1},\, \rho_1\,\big)}{\delta\rho} \\
& -f^{\text{eom}}\Big(\,\tau_1,\, q_1|_{\tau_1},\, h\big(q_1|_{\tau_1}, v_1|^-_{\tau_1}\big),\, \rho_1\,\Big)\,\frac{\delta\tau}{\delta\rho} \\
& +\frac{dh}{dq}\big(q_2|_{\tau_1}, v_2|_{\tau_1}\big)\cdot v_2|_{\tau_1}\cdot\frac{\delta\tau}{\delta\rho} + \frac{dh}{dv}\big(q_2|_{\tau_1}, v_2|_{\tau_1}\big)\cdot f^{\text{eom}}\Big(\,\tau_1,\, q_2|_{\tau_1},\, v_2|_{\tau_1},\, \rho_2\,\Big)\cdot\frac{\delta\tau}{\delta\rho} \\
\approx \quad & \frac{dh}{dt}\big(q_1|_{\tau_1}, v_1|^-_{\tau_1}\big)\cdot\frac{\tau_2-\tau_1}{\delta\rho} + \frac{dh}{dq}\big(q_1|_{\tau_1}, v_1|^-_{\tau_1}\big)\cdot\frac{q_2|_{\tau_1} - q_1|_{\tau_1}}{\delta\rho} + \frac{dh}{dv}\big(q_1|_{\tau_1}, v_1|^-_{\tau_1}\big)\cdot\frac{v_2|_{\tau_1} - v_1|^-_{\tau_1}}{\delta\rho} \\
& +\frac{dh}{d\rho}\big(q_1|_{\tau_1}, v_1|^-_{\tau_1}\big) - f^{\text{eom}}\Big(\tau_1,\, q_1|_{\tau_1},\; h\big(q_1|_{\tau_1}, v_1|^-_{\tau_1}\big),\, \rho_1\Big)\,\frac{\delta\tau}{\delta\rho} \\
& +\frac{dh}{dq}\big(q_2|_{\tau_1}, v_2|_{\tau_1}\big)\cdot v_2|_{\tau_1}\cdot\frac{\delta\tau}{\delta\rho} + \frac{dh}{dv}\big(q_2|_{\tau_1}, v_2|_{\tau_1}\big)\cdot f^{\text{eom}}\Big(\tau_1,\, q_2|_{\tau_1},\, v_2|_{\tau_1},\, \rho_2\Big)\cdot\frac{\delta\tau}{\delta\rho}.
\end{aligned}
$$

Taking the limit $\delta\rho \to 0$ *and using* (2.31) *yields:*

$$
\begin{aligned}
& \frac{dh}{dq}\big(q_1|_{\tau_1}, v_1|^-_{\tau_1}\big) \to h_q|^-_{t_{\text{eve}}}, \quad \frac{dh}{dq}\big(q_2|_{\tau_1}, v_2|_{\tau_1}\big) \to h_q|^-_{t_{\text{eve}}}, \\
& \frac{dh}{dv}\big(q_1|_{\tau_1}, v_1|^-_{\tau_1}\big) \to h_v|^-_{t_{\text{eve}}}, \quad \frac{dh}{dv}\big(q_2|_{\tau_1}, v_2|_{\tau_1}\big) \to h_v|^-_{t_{\text{eve}}}, \\
& \frac{dh}{dt}\big(q_1|_{\tau_1}, v_1|^-_{\tau_1}\big) \to h_t|^-_{t_{\text{eve}}}, \quad \frac{dh}{d\rho}\big(q_1|_{\tau_1}, v_1|^-_{\tau_1}\big) \to h_\rho|^-_{t_{\text{eve}}}, \\
& f^{\text{eom}}\Big(\tau_1,\, q_2|_{\tau_1},\, v_2|_{\tau_1},\, \rho_2\Big) \to f^{\text{eom}}\Big(t_{\text{eve}},\, q|^-_{t_{\text{eve}}},\, v|^-_{t_{\text{eve}}},\, \rho\Big) = \ddot{q}|^-_{t_{\text{eve}}}, \\
& f^{\text{eom}}\Big(\tau_1,\, q_1|_{\tau_1}, v_1|^+_{\tau_1},\, \rho_1\Big) \to f^{\text{eom}}\Big(t_{\text{eve}},\, q|^+_{t_{\text{eve}}},\, v|^+_{t_{\text{eve}}},\, \rho\Big) = \ddot{q}|^+_{t_{\text{eve}}}.
\end{aligned}
\tag{2.41}
$$

which leads to (2.38).

For simplicity we denote the derivatives of the jump function with respect to $\zeta \in \{t, q, v, \rho\}$

by:

$$\begin{aligned}\frac{dh}{d\zeta}\big(\tau_1,\, q_1|_{\tau_1},\, v_1|_{\tau_1}^-,\, \rho_1\,\big) &= \frac{dh}{d\zeta}\big(q_1|_{\tau_1}, v_1|_{\tau_1}^-\big)\\ \frac{dh}{d\zeta}\big(\tau_1,\, q_2|_{\tau_1},\, v_2|_{\tau_1},\, \rho_2\,\big) &= \frac{dh}{d\zeta}\big(q_2|_{\tau_1}, v_2|_{\tau_1}\big)\end{aligned} \tag{2.42}$$

□

Theorem 4 (Events that only change the acceleration)**.** *We now consider an event where the system undergoes a sudden change of the equation of motions* (2.1) *at* t_{eve}*. Let* $\ddot{q}|_{t_{\text{eve}}}^+$ *and* $\ddot{q}|_{t_{\text{eve}}}^- \in \mathbb{R}^n$ *be the generalized acceleration state vectors right after and right before the event, respectively:*

$$\ddot{q}|_{t_{\text{eve}}}^- \quad = f^{\text{eom}-}\big(t_{\text{eve}}, q|_{t_{\text{eve}}}, v|_{t_{\text{eve}}}, \rho\big) =: f^{\text{eom}-}|_{t_{\text{eve}}} \tag{2.43}$$

$$\xrightarrow{\text{event}} \quad \ddot{q}|_{t_{\text{eve}}}^+ \quad = f^{\text{eom}+}\big(t_{\text{eve}}, q|_{t_{\text{eve}}}, v|_{t_{\text{eve}}}, \rho\big) =: f^{\text{eom}+}|_{t_{\text{eve}}}. \tag{2.44}$$

There is no abrupt jump in the system velocity, $v|_{t_{\text{eve}}}^+ = v|_{t_{\text{eve}}}^-$*, and therefore the jump function* (2.27) *is identity. Let* $V|_{t_{\text{eve}}}^+, V|_{t_{\text{eve}}}^- \in \mathbb{R}^{n\times p}$ *be the sensitivities of the generalized position state vectors right after and before the event, respectively. The jump equation of the sensitivities of the generalized velocity state vector is:*

$$V|_{t_{\text{eve}}}^+ = V|_{t_{\text{eve}}}^- - \big(\ddot{q}|_{t_{\text{eve}}}^+ - \ddot{q}|_{t_{\text{eve}}}^-\big)\cdot\frac{dt_{\text{eve}}}{d\rho} = V|_{t_{\text{eve}}}^- - \big(f^{\text{eom}+}|_{t_{\text{eve}}} - f^{\text{eom}-}|_{t_{\text{eve}}}\big)\cdot\frac{dt_{\text{eve}}}{d\rho}. \tag{2.45}$$

Proof. *For the type of events under consideration we have that:*

$$\frac{dh}{dq} = \mathsf{0}, \quad \frac{dh}{dv} = \mathsf{I}. \tag{2.46}$$

Using this in (2.38) *leads to* (2.45). ☐

2.2.5 The jump in the sensitivity of the cost functional due to the event

We now consider the sensitivity of the quadrature variable $z(t)$. Due to the integral form of (2.7) defining z, the quadrature variable is continuous in time:

$$z|_{t_{\mathrm{eve}}}^{+} = z|_{t_{\mathrm{eve}}}^{-} = z|_{t_{\mathrm{eve}}}. \tag{2.47}$$

However, its sensitivity can be discontinuous at the event time, as established next.

Theorem 5 (Jump in quadrature sensitivity.)**.** *Let* $Z|_{t_{\mathrm{eve}}}^{+}$ *and* $Z|_{t_{\mathrm{eve}}}^{-}$*, with* $Z \in \mathbb{R}^p$*, be the sensitivities of the quadrature variable* $z(t)$ *(Definition 2.1.5) right after and right before the event, respectively. Let*

$$g|_{t_{\mathrm{eve}}}^{+} := \tilde{g}\big(t_{\mathrm{eve}}, q|_{t_{\mathrm{eve}}}, v|_{t_{\mathrm{eve}}}^{+}, \rho\big), \quad g|_{t_{\mathrm{eve}}}^{-} := \tilde{g}\big(t_{\mathrm{eve}}, q|_{t_{\mathrm{eve}}}, v|_{t_{\mathrm{eve}}}^{-}, \rho\big), \tag{2.48}$$

be the running cost function evaluated right after and right before the event, respectively. The *sensitivity of the cost functional changes during the event as follows:*

$$Z|_{t_{\rm eve}}^{+} = Z|_{t_{\rm eve}}^{-} - \left(g|_{t_{\rm eve}}^{+} - g|_{t_{\rm eve}}^{-} \right) \cdot \frac{dt_{\rm eve}}{d\rho}. \tag{2.49}$$

Proof. *Consider again the twin perturbed systems from Definition 2.2.3, and evaluate the associated quadrature variables* (2.7) *at the event:*

$$\begin{aligned} z_1|_{\tau_2} &= z_1|_{\tau_1} + \int_{\tau_1}^{\tau_2} \tilde{g}\big(t, q_1(t), v_1(t), \rho_1\big)\, dt = z_1|_{\tau_1} + \tilde{g}\big(\,\tau_1,\, q_1|_{\tau_1},\, v_1|_{\tau_1}^{+},\, \rho_1\,\big)\, \delta\tau, \\ z_2|_{\tau_2} &= z_2|_{\tau_1} + \int_{\tau_1}^{\tau_2} \tilde{g}\big(t, q_2(t), v_2(t), \rho_2\big)\, dt = z_2|_{\tau_1} + \tilde{g}\big(\,\tau_2,\, q_2|_{\tau_2},\, v_2|_{\tau_2}^{-},\, \rho_2\,\big)\, \delta\tau. \end{aligned} \tag{2.50}$$

Subtract the two equations and scale by the parameter perturbation to obtain:

$$\frac{z_2|_{\tau_2} - z_1|_{\tau_2}}{\delta\rho} = \frac{z_2|_{\tau_1} - z_1|_{\tau_1}}{\delta\rho} + \big(\tilde{g}\big(\,\tau_2,\, q_2|_{\tau_2},\, v_2|_{\tau_2}^{-},\, \rho_2\,\big) - \tilde{g}\big(\,\tau_1,\, q_1|_{\tau_1},\, v_1|_{\tau_1}^{+},\, \rho_1\,\big)\big)\, \frac{\delta\tau}{\delta\rho}. \tag{2.51}$$

Taking the limit $\delta\rho \to 0$ *leads to* (2.49). □

Remark. When there are multiple events along the trajectory jumps in sensitivity (2.49) will happen for each one. The jump of the quadrature variable Z is governed by the values of the cost function g before and after the event.

2.3 Direct sensitivity analysis for constrained multibody systems with smooth trajectories

This section reviews the direct sensitivity analysis for constrained systems governed by differential algebraic equations (DAEs). The presentation follows the authors' earlier work [58, 29, 1, 27, 2].

2.3.1 Representation of constrained multibody systems

Constrained multibody systems must satisfy the following kinematic constraints:

$$
\begin{aligned}
\mathsf{0} &= \Phi, && (2.52a)\\
\mathsf{0} &= \dot{\Phi} = \Phi_q\,\dot{q} + \Phi_t \quad \Rightarrow \quad \Phi_q v = -\Phi_t, && (2.52b)\\
\mathsf{0} &= \ddot{\Phi} = \Phi_q\,\ddot{q} + \Phi_{q,q}\,(\dot{q},\dot{q}) + \Phi_{t,q}\,\dot{q} + \Phi_{t,t} && (2.52c)\\
&\Rightarrow \Phi_q\,\dot{v} = -(\Phi_q\,v)\,v - \Phi_{t,q}\,v - \Phi_{t,t} := \mathsf{C}.
\end{aligned}
$$

Here (2.52a) is a holonomic position constraint equation $\Phi(t,q,\rho) = \mathsf{0}$, where $\Phi : \mathbb{R}^{1+n+p} \to \mathbb{R}^m$ is a smooth 'position constraint' function. The velocity (2.52b) and the acceleration (2.52c) kinematic constraints are found by differentiating the position constraint with respect to time.

There are two main approaches to solve such system, the DAE approach through direct inclusion of the algebraic constraints in the dynamics, and the ODE approach through either following locally the independent coordinates (Maggi) or through a penalty formulation.

2.3.2 Direct sensitivity analysis for smooth systems in the index-3 differential-algebraic formulation

Definition 2.3.1 (Constrained multibody dynamics: the index-3 DAE formulation)**.** A constrained rigid multibody dynamics system is described by the following index-3 differential-algebraic equations (DAEs) [58]:

$$\begin{cases} \dot{q} & = v, \\ \mathsf{M}\left(t,q,\rho\right) \cdot \dot{v} & = \mathsf{F}\left(t,q,v,\rho\right) + \Phi_q^{\mathrm{T}}\left(t,q,\rho\right) \cdot \mu, \qquad t_0 \le t \le t_F, \quad q(t_0) = q_0(\rho), \quad v(t_0) = v_0(\rho). \\ \Phi\left(t,q,\rho\right) & = 0, \end{cases} \tag{2.53}$$

Unlike the ODE formulation (2.2) the position vector of the system (2.53) is constrained by the equation (2.52a). The joint forces $\Phi_q^{\mathrm{T}}\,\mu$ ensure that the system solution obeys the constraints at all points along the trajectory, and $\mu \in \mathbb{R}^m$ are Lagrange multipliers associated with the position constraint (2.52a).

Sensitivities of the position and velocity state variables are defined in (2.3). In addition, we need to consider the sensitivity of the Lagrange multipliers with respect to system parameters:

$$\Lambda(t,\rho) := D_\rho \mu(t) := \frac{d\mu}{d\rho}(t,\rho) \in \mathbb{R}^{m\times p}. \tag{2.54}$$

Definition 2.3.2 (TLM of the index-3 DAE formulation)**.** Sensitivities of solutions (2.3) and multipliers (2.54) of the system (2.53) with respect to parameters evolve according to the tangent linear model derived in [58, 29, 1, 27, 2]:

$$\begin{cases} \dot{Q} = V, \\ \mathsf{M}\cdot\dot{V} = \mathsf{F}_v\cdot V - \left(\mathsf{M}_q\,\dot{v} + \Phi_{q,q}^{\mathrm{T}}\,\mu - \mathsf{F}_q\right)\cdot Q - \Phi_q^{\mathrm{T}}\cdot\Lambda + \mathsf{F}_\rho - \mathsf{M}_\rho\,\dot{v} - \Phi_{q,\rho}^{\mathrm{T}}\mu, \\ \Phi_q\cdot Q = -\Phi_\rho, \end{cases} \tag{2.55}$$

with initial conditions given by (2.14b).

2.3.3 Direct sensitivity analysis for smooth systems in the index-1 differential-algebraic formulation

Definition 2.3.3 (Constrained multibody dynamics: the index-1 DAE formulation)**.** The index-1 formulation of the equations of motion is obtained by replacing the position constraint (2.52a) in (2.53) with the acceleration constraint (2.52c):

$$\begin{bmatrix} \mathsf{I} & 0 & 0 \\ 0 & \mathsf{M}\,(t,q,\rho) & \Phi_q^{\mathrm{T}}\,(t,q,\rho) \\ 0 & \Phi_q\,(t,q,\rho) & 0 \end{bmatrix} \cdot \begin{bmatrix} \dot{q} \\ \dot{v} \\ \mu \end{bmatrix} = \begin{bmatrix} v \\ \mathsf{F}\,(t,q,v,\rho) \\ \mathsf{C}\,(t,q,v,\rho) \end{bmatrix}, \quad t_0 \le t \le t_F, \quad q(t_0) = q_0(\rho), \quad v(t_0) = v_0(\rho), \tag{2.56}$$

or equivalently,

$$\dot{q} = v, \qquad \begin{bmatrix} \dot{v} \\ \mu \end{bmatrix} = \begin{bmatrix} \mathsf{M} & \Phi_q^{\mathrm{T}} \\ \Phi_q & 0 \end{bmatrix}^{-1} \cdot \begin{bmatrix} \mathsf{F} \\ \mathsf{C} \end{bmatrix} = \begin{bmatrix} f^{\text{DAE-}\dot{v}} \\ f^{\text{DAE-}\mu} \end{bmatrix} = f^{\text{DAE}}(\,t,\, q,\, v,\, \rho\,). \tag{2.57}$$

The algebraic equation has the form $f^{\text{DAE-}\mu} - \mu = 0$.

Definition 2.3.4 (TLM of the index-1 DAE formulation)**.** Sensitivities of solutions (2.3) and multipliers (2.54) of the system (2.56) with respect to parameters evolve according to the tangent linear model derived in [58, 29, 1, 27, 2]:

$$\begin{bmatrix} \mathsf{I} & 0 & 0 \\ 0 & \mathsf{M} & \Phi_q^{\mathrm{T}} \\ 0 & \Phi_q & 0 \end{bmatrix} \cdot \begin{bmatrix} \dot{Q} \\ \dot{V} \\ \mu \end{bmatrix} = \begin{bmatrix} V \\ \mathsf{F}_v \cdot V - \left(\mathsf{M}_q\,\dot{v} + \Phi_{q,\,q}^{\mathrm{T}}\,\mu - \mathsf{F}_q\right) \cdot Q + \mathsf{F}_\rho - \mathsf{M}_\rho\,\dot{v} - \Phi_{q,\,\rho}^{\mathrm{T}}\,\mu \\ \mathsf{C}_v \cdot V - \left(\Phi_{q,\,q}\,\dot{v} - \mathsf{C}_q\right) \cdot Q + \mathsf{C}_\rho - \Phi_{q,\,\rho}\,\dot{v} \end{bmatrix}, \tag{2.58}$$

with initial conditions given by (2.14b).

Definition 2.3.5 (Cost function)**.** Following Definition 2.3.4, consider a smooth scalar "trajectory cost function" g and a smooth scalar "terminal cost function" w. A general cost function has the form:

$$\psi = \int_{t_0}^{t_F} g\big(\, t,\, q(t,\rho),\, v(t,\rho),\, \dot{v}(t,\rho),\, \mu(t,\rho),\, \rho\,\big)\ dt + w\big(t_F, q(t_F,\rho), v(t_F,\rho), \rho\big).$$

Note that the trajectory cost function (2.5) depends on both accelerations $\dot{v}$ and on the Lagrange multipliers μ. These are not independent variables and they can be resolved in terms of positions and velocities using (2.56), to obtain an equivalent regular trajectory cost function:

$$g\big(\, t,\, q,\, v,\, \dot{v}(t,q,v,\rho),\, \mu(t,q,v,\rho),\, \rho\,\big) = \tilde{g}\big(\, t,\, q,\, v,\, \rho\,\big). \tag{2.59}$$

We keep accelerations and Lagrange multipliers (constraint forces) as explicit parameters in the cost function (2.59) in order to give additional flexibility in practical applications. In addition, we define the 'quadrature' variable $z(t) \in \mathbb{R}$ as follows:

$$\begin{aligned} z(t,\rho) &:= \int_{t_0}^{t} \tilde{g}\big(t, q(t,\rho), v(t,\rho), \rho\big)\, dt \quad \Leftrightarrow && \text{(2.60a)} \\ \dot{z}(t,\rho) &= g\big(\, t,\, q,\, v,\, \dot{v},\, \mu,\, \rho\,\big) = \tilde{g}\big(t, q(t,\rho), v(t,\rho), \rho\big), && \text{(2.60b)} \\ & \qquad t_0 \le t \le t_F, \quad z(t_0,\rho) = 0. \end{aligned}$$

Definition 2.3.6 (The DAE quadrature sensitivity)**.** Similarly, let the 'quadrature sensitivity' vector $Z(t,\rho)$ be the Jacobian of the 'quadrature' variable $z(t,\rho)$ (2.60a) with respect to the parameters ρ:

$$Z_i(t,\rho) := \frac{\partial z(t,\rho)}{\partial \rho_i}, \quad i = 1,\ldots,p; \quad Z(t,\rho) := \nabla_\rho z(t,\rho) = \Big[Z_1(t,\rho) \cdots Z_p(t,\rho) \Big] \in \mathbb{R}^{1\times p}. \tag{2.61}$$

The time evolution equations of the quadrature sensitivities are given by the TLM obtained by differentiating (2.60b) with respect to the parameters:

$$\begin{aligned}
\dot{Z}_i &= \frac{d\,g\big(t,\,q,\,v,\,\dot{v},\,\mu,\,\rho\big)}{d\,\rho_i} \\
&= g_q \cdot Q_i + g_v \cdot V_i + g_{\dot{v}} \cdot \frac{d f^{\mathrm{DAE}\text{-}\dot{v}}}{d\rho} + g_\mu \cdot \frac{d f^{\mathrm{DAE}\text{-}\mu}}{d\rho} + g_{\rho_i} \\
&= \big(g_q + g_{\dot{v}} \cdot f_q^{\mathrm{DAE}\text{-}\dot{v}} + g_\mu \cdot f_q^{\mathrm{DAE}\text{-}\mu}\big) \cdot Q_i + \big(g_v + g_{\dot{v}} \cdot f_v^{\mathrm{DAE}\text{-}\dot{v}} + g_\mu \cdot f_v^{\mathrm{DAE}\text{-}\mu}\big) \cdot V_i + \big(g_{\rho_i} + g_{\dot{v}} \cdot f_{\rho_i}^{\mathrm{DAE}\text{-}\dot{v}} + g_\mu \cdot f_{\rho_i}^{\mathrm{DAE}\text{-}\mu}\big), \\
&= \tilde{g}_q \cdot Q_i + \tilde{g}_v \cdot V_i + \tilde{g}_{\rho_i}, \\
&= \frac{d\,\tilde{g}\big(t,\,q,\,v,\,\rho\big)}{d\,\rho_i}, \\
& i = 1,\ldots,p, \quad t_0 \le t \le t_F, \quad Z_i(t_0,\rho) = 0.
\end{aligned} \tag{2.62}$$

Definition 2.3.7 (Canonical index-1 sensitivity DAE)**.** The canonical DAE system for the solution given by (2.57), the DAE TLM given by (2.58), and the sensitivity quadrature equations given by (2.62) need to be solved together forward in time, leading to the canonical sensitivity DAE that computes the derivatives of the cost function with respect to the system parameters ρ for smooth systems:

$$\begin{bmatrix} \dot{q} \\ \dot{v} \\ \mu \\ \dot{z} \\ \left[\dot{Q}_i\right]_{i=1,\dots,p} \\ \left[\dot{V}_i\right]_{i=1,\dots,p} \\ \left[\Lambda_i\right]_{i=1,\dots,p} \\ \left[\dot{Z}_i\right]_{i=1,\dots,p} \end{bmatrix} = \begin{bmatrix} v \\ f^{\text{DAE-}\dot{v}} \\ f^{\text{DAE-}\mu} \\ \tilde{g} \\ \left[V_i\right]_{i=1,\dots,p} \\ \left[f_q^{\text{DAE-}\dot{v}} Q_i + f_v^{\text{DAE-}\dot{v}} V_i + f_{\rho_i}^{\text{DAE-}\dot{v}}\right]_{i=1,\dots,p} \\ \left[f_q^{\text{DAE-}\mu} Q_i + f_v^{\text{DAE-}\mu} V_i + f_{\rho_i}^{\text{DAE-}\mu}\right]_{i=1,\dots,p} \\ \left[\tilde{g}_q \cdot Q_i + \tilde{g}_v \cdot V_i + \tilde{g}_{\rho_i}\right]_{i=1,\dots,p} \end{bmatrix}, \tag{2.63}$$

where the state vector of the canonical index-1 sensitivity DAE (2.63) is :

$$X = \left[\, q^{\mathrm{T}},\, v^{\mathrm{T}}, \mu^{\mathrm{T}},\, z,\; Q_1^{\mathrm{T}}, \dots, Q_p^{\mathrm{T}},\, V_1^{\mathrm{T}}, \dots, V_p^{\mathrm{T}},\, \Lambda_1^{\mathrm{T}}, \dots, \Lambda_p^{\mathrm{T}},\, Z_1, \dots, Z_p \right]^{\mathrm{T}} \in \mathbb{R}^{(n+1)(p+1)} \tag{2.64}$$

and the derivatives of the DAE function are:

$$f_q^{\text{DAE}} = \begin{bmatrix} \mathsf{M} & \Phi_q^{\mathrm{T}} \\ \Phi_q & 0 \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{F}_q - \mathsf{M}_q\, \dot{v} - \Phi_{q,\,q}^{\mathrm{T}}\, \mu \\ \mathsf{C}_q - \Phi_{q,\,q} \dot{v} \end{bmatrix},\; f_v^{\text{DAE}} = \begin{bmatrix} \mathsf{M} & \Phi_q^{\mathrm{T}} \\ \Phi_q & 0 \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{F}_v \\ \mathsf{C}_v \end{bmatrix} \tag{2.65a}$$

$$f_\rho^{\text{DAE}} = \begin{bmatrix} \mathsf{M} & \Phi_q^{\mathrm{T}} \\ \Phi_q & 0 \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{F}_\rho - \mathsf{M}_\rho\, \dot{v} - \Phi_{q,\,\rho}^{T}\, \mu \\ \mathsf{C}_\rho - \Phi_{q,\,\rho}\, \dot{v} \end{bmatrix}. \tag{2.65b}$$

2.3.4 Direct sensitivity analysis for smooth systems in the penalty ODE formulation

Definition 2.3.8 (Constrained multibody dynamics systems: the penalty ODE formulation)**.** Define the extended mass matrix $\overline{\mathsf{M}} : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^{n \times n}$ as:

$$\overline{\mathsf{M}}\,(t, q, v, \rho) := \mathsf{M}\,(t, q, v, \rho) + \Phi_q^{\mathrm{T}}\,(t, q, v, \rho) \cdot \alpha \cdot \Phi_q\,(t, q, v, \rho)\,, \tag{2.66a}$$

where $\alpha \in \mathbb{R}^{m \times m}$ is the penalty factor of the ODE penalty formulation. Define the extended right-hand side function $\overline{\mathsf{F}} : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^n$ as:

$$\overline{\mathsf{F}}\,(t, q, v, \rho) := \mathsf{F}\,(t, q, v, \rho) - \Phi_q^{\mathrm{T}} \cdot \alpha \cdot \Big(\dot{\Phi}_q\, v + \dot{\Phi}_t + 2\,\xi\,\omega\,\dot{\Phi} + \omega^2 \Phi\Big)\,, \tag{2.66b}$$

where $\xi \in \mathbb{R}$ and $\omega \in \mathbb{R}$ are the natural frequency and damping ratio coefficients of the formulation, respectively, and $\dot{\Phi}$ is the total time derivative of the kinematic constraints. The algebraic position constraints (2.52a) are removed and an auxiliary spring-damper force is added in (2.66b) to prevent the system from deviating away from the constraints.

In the penalty formulation the EOM of a constrained rigid multibody system is the second order ODE:

$$\begin{cases} \dot{q} & = v, \\ \dot{v} & = f^{\mathrm{eom}}(\,t,\, q,\, v,\, \rho\,) = \overline{\mathsf{M}}^{-1}(\,t,\, q,\, v,\, \rho\,) \cdot \overline{\mathsf{F}}(\,t,\, q,\, v,\, \rho\,). \end{cases} \tag{2.66c}$$

The Lagrange multipliers associated to the constraint forces are estimated as follows:

$$\mu^{*} = \alpha \left(\ddot{\Phi} + 2\,\xi\,\omega\,\dot{\Phi} + \omega^{2}\,\Phi \right) . \tag{2.66d}$$

The cost function (2.59) is formulated using the Lagrange multiplier estimates (2.66d), i.e., using the trajectory cost function $g\,(\,t,\,q,\,v,\,\dot{v},\,\mu^{*},\,\rho\,)$. Sensitivities (2.3) of the position and velocity state variables of the system (2.66) with respect to parameters evolve according to the tangent linear model derived in [58, 29, 1, 27, 2]:

$$\begin{cases} \dot{Q} &= V, \\ \overline{\mathsf{M}} \cdot \dot{V} &= \left(\overline{\mathsf{F}}_{q} - \overline{\mathsf{M}}_{q}\,\dot{v} \right) \cdot Q + \overline{\mathsf{F}}_{v} \cdot V + \overline{\mathsf{F}}_{\rho} - \overline{\mathsf{M}}_{\rho}\,\dot{v}, \end{cases} \qquad t_{0} \le t \le t_{F}, \tag{2.67}$$

with initial conditions given by (2.14b). The derivatives $\overline{\mathsf{F}}_{q}, \overline{\mathsf{F}}_{v}, \overline{\mathsf{F}}_{\rho}, \overline{\mathsf{M}}_{\rho}$, and $\overline{\mathsf{M}}_{q}$ are given in A.

Definition 2.3.9 (The canonical ODE sensitivity)**.** The canonical sensitivity ODE that computes the derivatives of the cost function with respect to the system parameters ρ for the smooth ODE penalty system (2.66) is the same than the ODE canonical system presented in (2.18) and extended to the cost function (2.59) formulated using the Lagrange multiplier estimates.

$$\begin{bmatrix} \dot{q} \\ \dot{v} \\ \dot{z} \\ \left[\dot{Q}_i\right]_{i=1,\ldots,p} \\ \left[\dot{V}_i\right]_{i=1,\ldots,p} \\ \left[\dot{Z}_i\right]_{i=1,\ldots,p} \end{bmatrix} = \begin{bmatrix} v \\ f^{\text{eom}} \\ \tilde{g} \\ \left[V_i\right]_{i=1,\ldots,p} \\ \left[f_q^{\text{eom}} \cdot Q_i + f_v^{\text{eom}} \cdot V_i + f_{\rho_i}^{\text{eom}}\right]_{i=1,\ldots,p} \\ \left[\tilde{g}_q \cdot Q_i + \tilde{g}_v \cdot V_i + \tilde{g}_{\rho_i}\right]_{i=1,\ldots,p} \end{bmatrix}, \tag{2.68}$$

where

$$\tilde{g}_q \cdot Q_i + \tilde{g}_v \cdot V_i + \tilde{g}_{\rho_i} = \left(g_q + g_{\dot{v}} \cdot f_q^{\text{eom}} + g_{\mu^*} \cdot \mu_q^*\right) \cdot Q_i + \left(g_v + g_{\dot{v}} \cdot f_v^{\text{eom}} + g_{\mu^*} \cdot \mu_v^*\right) \cdot V_i + \left(g_{\rho_i} + g_{\dot{v}} \cdot f_{\rho_i}^{\text{eom}} + g_{\dot{v}} \cdot \mu_\rho^*\right) \tag{2.69}$$

and

$$f_q^{\text{eom}} = \overline{\mathsf{M}}^{-1}\left(\overline{\mathsf{F}}_q - \overline{\mathsf{M}}_q \dot{v}\right), \quad f_v^{\text{eom}} = \overline{\mathsf{M}}^{-1}\overline{\mathsf{F}}_v, \quad f_{\rho_i}^{\text{eom}} = \overline{\mathsf{M}}^{-1}\left(\overline{\mathsf{F}}_\rho - \overline{\mathsf{M}}_\rho \dot{v}\right), \tag{2.70}$$

and with the initial conditions given by (2.14b). The derivatives μ_q^*, μ_v^* and μ_ρ^* are given in A.

Remark. The sensitivity of the estimated Lagrange multipliers

$$\Lambda^*(t, \rho) := D_\rho \mu^*(t) := \frac{d\mu^*}{d\rho}(t, \rho) \in \mathbb{R}^{m \times p} \tag{2.71}$$

is calculated as:

$$\Lambda_i^* = \mu_q^* \, Q_i + \mu_v^* \, V_i + \mu_{\rho_i}^*, \quad i = 1, \ldots, p. \tag{2.72}$$

2.4 Direct sensitivity analysis for hybrid constrained multibody systems

We now discuss constrained multibody systems when the dynamics is piecewise continuous in time.

2.4.1 Coordinates partitioning for hybrid multibody systems

The direct sensitivity analysis for a constrained rigid hybrid multibody dynamic system requires to find the jump conditions at the time of event. For this we need to distinguish between dependent and independent state variables and their sensitivities.

Assume that the Jacobian of the position constraint (2.52a) has full row rank at a given configuration, $\mathrm{rank}(\Phi_q) = m$. One can rearrange the columns and split the Jacobian in two submatrices:

$$\Phi_q \cdot \mathsf{P}^{\mathrm{T}} = \begin{bmatrix} \Phi_{q_{\mathrm{dep}}} & \Phi_{q_{\mathrm{dof}}} \end{bmatrix}, \quad \Phi_{q_{\mathrm{dep}}} \in \mathbb{R}^{m \times m}, \quad \Phi_{q_{\mathrm{dof}}} \in \mathbb{R}^{m \times f}, \quad f = n - m, \tag{2.73}$$

such that the first block $\Phi_{q_{\mathrm{dep}}}$ is nonsingular. Here $\mathsf{P} \in \mathbb{R}^{n \times n}$ is a permutation matrix, obtained by permuting rows of identity matrix; the multiplication $\Phi_q \cdot \mathsf{P}$ performs a permutation of the columns of Φ_q.

By the implicit function theorem one can partition locally the position state variables into independent coordinates $q_{\rm dof} \in \mathbb{R}^f$ (the local 'degrees of freedom' of the system) and dependent coordinates $q_{\rm dep} \in \mathbb{R}^m$, and solve for the dependent ones in terms of the degrees of freedom:

$$\Phi(t,q) = \mathsf{0} \quad \text{and} \quad \Phi_{q_{\rm dep}}(t,q) \text{ nonsingular} \quad \Rightarrow \quad q_{\rm dep} = \zeta\big(t, q_{\rm dof}\big). \tag{2.74}$$

This induces a corresponding local partitioning of the state variables into independent components $q_{\rm dof}, v_{\rm dof} \in \mathbb{R}^f$ and dependent components $q_{\rm dep}, v_{\rm dep} \in \mathbb{R}^m$:

$$\mathsf{P} \cdot q = \begin{bmatrix} \mathsf{P}_{\rm dep} \\ \mathsf{P}_{\rm dof} \end{bmatrix} \cdot q = \begin{bmatrix} q_{\rm dep} \\ q_{\rm dof} \end{bmatrix}, \qquad \mathsf{P} \cdot v = \begin{bmatrix} \mathsf{P}_{\rm dep} \\ \mathsf{P}_{\rm dof} \end{bmatrix} \cdot v = \begin{bmatrix} v_{\rm dep} \\ v_{\rm dof} \end{bmatrix}, \tag{2.75}$$

where $\mathsf{P}_{\rm dep} \in \mathbb{R}^{m \times n}$ and $\mathsf{P}_{\rm dof} \in \mathbb{R}^{f \times n}$ consist the first m and the last f rows of P, respectively. Let:

$$\mathsf{R} := -\Phi_{q_{\rm dep}}^{-1}\, \Phi_{q_{\rm dof}} \in \mathbb{R}^{m \times f}. \tag{2.76}$$

The velocity constraint equation (2.52b) becomes:

$$\Phi_{q_{\rm dep}}\, v_{\rm dep} + \Phi_{q_{\rm dof}}\, v_{\rm dof} = -\Phi_t \quad \Rightarrow \quad v_{\rm dep} = -\Phi_{q_{\rm dep}}^{-1} \left(\Phi_{q_{\rm dof}}\, v_{\rm dof} + \Phi_t\right) = \mathsf{R}\, v_{\rm dof} - \Phi_{q_{\rm dep}}^{-1}\, \Phi_t. \tag{2.77}$$

Similarly, the acceleration constraint equation (2.52c) becomes:

$$\Phi_{q_{\mathrm{dep}}}\,\dot{v}_{\mathrm{dep}} + \Phi_{q_{\mathrm{dof}}}\,\dot{v}_{\mathrm{dof}} = \mathsf{C} \quad \Rightarrow \quad \dot{v}_{\mathrm{dep}} = -\Phi_{q_{\mathrm{dep}}}^{-1}\left(\Phi_{q_{\mathrm{dof}}}\,\dot{v}_{\mathrm{dof}} - \mathsf{C}\right) = \mathsf{R}\,\dot{v}_{\mathrm{dof}} + \Phi_{q_{\mathrm{dep}}}^{-1}\,\mathsf{C}. \tag{2.78}$$

From (2.73), (2.75), and (2.76) we have that:

$$\Phi_{q_{\mathrm{dof}}} = \Phi_q \cdot \mathsf{P}_{\mathrm{dof}}^{\mathrm{T}} \in \mathbb{R}^{m\times f}, \quad \Phi_{q_{\mathrm{dep}}} = \Phi_q \cdot \mathsf{P}_{\mathrm{dep}}^{\mathrm{T}} \in \mathbb{R}^{m\times m}, \quad \mathsf{R} = -\left(\Phi_q \cdot \mathsf{P}_{\mathrm{dep}}^{\mathrm{T}}\right)^{-1} \cdot \Phi_q \cdot \mathsf{P}_{\mathrm{dof}}^{\mathrm{T}}. \tag{2.79}$$

2.4.2 Representation of constrained hybrid multibody systems

The hybrid dynamics of a constrained mechanical system refers to the smooth system defined in Section 2.3 subjected to a finite number of events, as discussed in Definition 2.2.1. Each event (2.24) happening at the 'time of event' t_{eve} introduces a kink in the trajectory of the mechanical system. At each event the velocity state vector of an *unconstrained* system undergoes a jump (2.27) that can be arbitrary, i.e., can be described by any smooth function $h(\cdot)$. In case of a *constrained* system we need a more comprehensive understanding of the event.

Definition 2.4.1 (Characterization of an event for constrained multibody systems)**.** During an event at time t_{eve} a constrained mechanical system undergoes a sudden change in state characterized as follows:

- The constraints may change at the time of event (e.g., when a walking humanoid robot changes its supporting foot at each step). Consequently, the position constraint function (2.52a) changes from $\Phi^- : \mathbb{R}^{1+n+p} \to \mathbb{R}^{m-}$ before event to $\Phi^+ : \mathbb{R}^{1+n+p} \to \mathbb{R}^{m+}$ after event:

$$\Phi^-(t,q,\rho) \xrightarrow{\text{event}} \Phi^+(t,q,\rho).$$

The two constraint functions are different, and in particular the number of constraints can differ, $m^+ \neq m^-$.

- The Jacobians of the position constraints before and after the event have full row ranks at the event configuration $q|_{t_{\text{eve}}}$:

$$\operatorname{rank}\left(\Phi_q^-(t,q,\rho)\right) = m^-, \quad \operatorname{rank}\left(\Phi_q^+(t,q,\rho) = m^+. \tag{2.80}$$

- Since the constraints can be different after and before the event, the partitions of variables into independent and dependent can also differ. We denote by $\square_{\text{dof-}}, \square_{\text{dep-}}$ the independent and dependent components before the event, and by $\square_{\text{dof+}}, \square_{\text{dep+}}$ the independent and dependent components after the event:

$$\mathsf{P}^- \cdot v = \begin{bmatrix} v_{\text{dep-}} \\ v_{\text{dof-}} \end{bmatrix} \in \mathbb{R}^n, \quad v_{\text{dof-}} \in \mathbb{R}^{f-}, \qquad \mathsf{P}^+ \cdot v = \begin{bmatrix} v_{\text{dep+}} \\ v_{\text{dof+}} \end{bmatrix} \in \mathbb{R}^n, \quad v_{\text{dof+}} \in \mathbb{R}^{f+}. \tag{2.81}$$

Here P^- and P^+ are the permutation matrices that select the dependent and independent coordinates before and after the event, respectively. The dimensions of the velocity degrees of freedom vectors are $f^- = n - m^-$ and $f^+ = n - m^+$ before and after the event, respectively.

- The generalized position state variables remain the same (2.26), i.e., $q|_{t_{\rm eve}}^{+} = q|_{t_{\rm eve}}^{-} = q|_{t_{\rm eve}}$. Consequently, the state at the time of event $q|_{t_{\rm eve}}$ need to satisfy both constraint functions:

$$\Phi^-|_{t_{\rm eve}}^- := \Phi^-\left(t_{\rm eve}, q|_{t_{\rm eve}}, \rho\right) = 0, \qquad \Phi^+|_{t_{\rm eve}}^+ := \Phi^+\left(t_{\rm eve}, q|_{t_{\rm eve}}, \rho\right) = 0. \tag{2.82}$$

At the event the system moves from one constraint manifold to another, and $q|_{t_{\rm eve}}$ is on the intersection of the two manifolds.

- The jump in velocity from right before the event to right after the event is defined in terms of the independent components, i.e., in terms of the velocity degrees of freedom:

$$v_{\text{dof+}}|_{t_{\rm eve}}^+ = h\Big(t_{\rm eve}, q|_{t_{\rm eve}}, v_{\text{dof-}}|_{t_{\rm eve}}^-, \rho\Big), \qquad h : \mathbb{R}^{1+n+f^-+p} \to \mathbb{R}^{f^+}. \tag{2.83}$$

The jump function (2.83) is assumed to be smooth. Note that its formulation is not unique, since it depends on the selections of the degrees of freedom that are not unique.

- The velocity state vectors satisfy the velocity kinematic constraints (2.77). Consequently, the jumps in velocity (2.27) cannot be arbitrary for the dependent components. The dependent components of velocity are obtained from solving the velocity constraints (2.77):

$$\begin{aligned} v_{\mathrm{dep}+}|_{t_{\mathrm{eve}}}^{+} &= -\left(\Phi_{q_{\mathrm{dep}+}}^{+}|_{t_{\mathrm{eve}}}^{+}\right)^{-1} \cdot \left(\Phi_{q_{\mathrm{dof}+}}^{+}|_{t_{\mathrm{eve}}}^{+}\, v_{\mathrm{dof}+}|_{t_{\mathrm{eve}}}^{+} + \Phi_{t}^{+}|_{t_{\mathrm{eve}}}^{+}\right) \\ &= \mathsf{R}^{+}|_{t_{\mathrm{eve}}}^{+}\, v_{\mathrm{dof}+}|_{t_{\mathrm{eve}}}^{+} - \left(\Phi_{q_{\mathrm{dep}+}}^{+}|_{t_{\mathrm{eve}}}^{+}\right)^{-1} \cdot \Phi_{t}^{+}|_{t_{\mathrm{eve}}}^{+}. \end{aligned} \tag{2.84}$$

Here $\mathsf{R}^{\pm}$ are the matrices corresponding to the constraints $\Phi^{\pm}$.

Remark (Collision events). The proposed formalism (2.83)–(2.84) covers the case of elastic contact/collision/impact without change in the set of constraint equations, $\Phi^{+} \equiv \Phi^{-}$. The impulsive (external) contact forces act to change the independent components of the velocity state (2.83).

Remark (Hybrid DAE jump formulation). The proposed formalism (2.83)–(2.84) also covers the case where the event consists solely of a change of constraints $\Phi^{+} \neq \Phi^{-}$, without any external force to modify the independent velocities. This type of event appears mainly in the humanoid robotics field where general and relative coordinates are used and inelastic collisions are considered. A popular approach in robotics is to solve for the DAE involving impulsive forces in the constraints at the time of event [31]:

$$\begin{bmatrix} \mathsf{M}|_{t_{\mathrm{eve}}} & (\Phi_{q}^{+})^{\mathrm{T}}|_{t_{\mathrm{eve}}} \\ \Phi_{q}^{+}|_{t_{\mathrm{eve}}} & \mathsf{0} \end{bmatrix} \cdot \begin{bmatrix} v|_{t_{\mathrm{eve}}}^{+} \\ \delta\mu \end{bmatrix} = \begin{bmatrix} \mathsf{M}|_{t_{\mathrm{eve}}} \cdot v|_{t_{\mathrm{eve}}}^{-} \\ -\Phi_{t}^{+}|_{t_{\mathrm{eve}}} \end{bmatrix}, \tag{2.85a}$$

or equivalently,

$$\begin{bmatrix} v|^{+}_{t_{\rm eve}} \\ \\ \delta\mu \end{bmatrix} = \begin{bmatrix} \mathsf{M}|_{t_{\rm eve}} & (\Phi^{+}_{q})^{\rm T}|_{t_{\rm eve}} \\ \\ \Phi^{+}_{q}|_{t_{\rm eve}} & \mathsf{0} \end{bmatrix}^{-1} \cdot \begin{bmatrix} \mathsf{M}|_{t_{\rm eve}} \cdot v|^{-}_{t_{\rm eve}} \\ \\ -\Phi^{+}_{t}|_{t_{\rm eve}} \end{bmatrix} = \begin{bmatrix} f^{\text{DAE-imp-}v}\big(t_{\rm eve},\, q|_{t_{\rm eve}},\, v|^{-}_{t_{\rm eve}},\, \rho\big) \\ \\ f^{\text{DAE-imp-}\mu}\big(t_{\rm eve},\, q|_{t_{\rm eve}},\, v|^{-}_{t_{\rm eve}},\, \rho\big) \end{bmatrix}. \tag{2.85b}$$

Here $v|^{+}_{t_{\rm eve}}$ contains both the independent and dependent coordinates. We see that the second equation in (2.85a) automatically imposes the velocity constraint (2.52b).

Our formalism covers this approach by defining the jump function given by (2.83) as:

$$v_{\rm dof+}|^{+}_{t_{\rm eve}} = \mathsf{P}_{\rm dof+}\, f^{\text{DAE-imp-}v}\big(t_{\rm eve},\, q|_{t_{\rm eve}},\, v|^{-}_{t_{\rm eve}},\, \rho\big) =: h\left(t_{\rm eve},\, q|_{t_{\rm eve}},\, v_{\rm dof-}|^{-}_{t_{\rm eve}},\, \rho\right). \tag{2.86}$$

2.4.3 The jump in the sensitivity of the position state vector

The jump conditions at the time of event in the sensitivity state vector for a constrained rigid multibody involve finding the sudden change in values of the sensitivity with respect to the system parameters ρ of the position and the dependent and independent velocity state variables due the impulsive jump of the independent velocity state variables.

Remark (Partitioning of sensitivity matrices). The partitioning of state variables into dependent and independent (2.81) induces a similar partitioning of the sensitivity matrices (2.3):

$$\mathsf{P} \cdot Q = \begin{bmatrix} Q_{\text{dep}} \\ Q_{\text{dof}} \end{bmatrix} \in \mathbb{R}^{n \times p}, \quad Q_{\text{dof}} \in \mathbb{R}^{f \times p}, \qquad \mathsf{P} \cdot V = \begin{bmatrix} V_{\text{dep}} \\ V_{\text{dof}} \end{bmatrix} \in \mathbb{R}^{n \times p}, \quad V_{\text{dof}} \in \mathbb{R}^{f \times p}. \tag{2.87}$$

Differentiation of the position constraint equation (2.52a) with respect to the system parameters ρ gives:

$$\mathsf{0} = \frac{d\Phi(t, q(t,\rho), \rho)}{d\rho} = \Phi_q \cdot Q + \Phi_\rho = \Phi_{q_{\text{dep}}} \cdot Q_{\text{dep}} + \Phi_{q_{\text{dof}}} \cdot Q_{\text{dof}} + \Phi_\rho, \tag{2.88}$$

and therefore:

$$Q_{\text{dep}} = -\Phi_{q_{\text{dep}}}^{-1} \left(\Phi_{q_{\text{dof}}} \cdot Q_{\text{dof}} + \Phi_\rho\right) = \mathsf{R} \cdot Q_{\text{dof}} - \Phi_{q_{\text{dep}}}^{-1} \Phi_\rho. \tag{2.89}$$

Similarly, differentiation of the velocity constraint equation (2.52b) with respect to the system parameters gives:

$$\begin{aligned} \mathsf{0} &= \frac{d}{d\rho} \left(\Phi_q(t, q(t,\rho), \rho)\, v(t,\rho) + \Phi_t(t, q(t,\rho), \rho)\right) \\ &= \Phi_q \cdot V + \left(\Phi_{q,q}\, v + \Phi_{q,t}\right) \cdot Q + \Phi_{\rho,q}\, v + \Phi_{\rho,t} \\ &= \Phi_{q_{\text{dep}}} \cdot V_{\text{dep}} + \Phi_{q_{\text{dof}}} \cdot V_{\text{dof}} + \Big(\Phi_{q,q}\, v + \Phi_{q,t}\Big) \cdot Q + \Phi_{\rho,q}\, v + \Phi_{\rho,t}, \end{aligned}$$

and therefore:

$$V_{\text{dep}} = \mathsf{R} \cdot V_{\text{dof}} - \Phi_{q_{\text{dep}}}^{-1} \left(\left(\Phi_{q,q}\, v + \Phi_{q,t} \right) \cdot Q + \Phi_{\rho,q}\, v + \Phi_{\rho,t} \right) . \tag{2.90}$$

Remark (Sensitivity of the time of event for constrained systems). The time of event depends only on the position state and on the event function (2.24). Consequently, the sensitivity of the time of event for constrained systems is the same as for unconstrained systems, and is given by (2.33) in Theorem 1.

Theorem 6 (Jump in position sensitivity for constrained systems)**.** *Let* $Q|_{t_{\text{eve}}}^{+}$ *and* $Q|_{t_{\text{eve}}}^{-} \in \mathbb{R}^{n \times p}$ *be the sensitivities of the generalized position state vectors right after and right before the event, respectively. The independent components of the sensitivity of the generalized positions right after the event are:*

$$Q_{\text{dof+}}|_{t_{\text{eve}}}^{+} = Q_{\text{dof+}}|_{t_{\text{eve}}}^{-} - \left(v_{\text{dof+}}|_{t_{\text{eve}}}^{+} - v_{\text{dof+}}|_{t_{\text{eve}}}^{-} \right) \cdot \frac{dt_{\text{eve}}}{d\rho}. \tag{2.91a}$$

The dependent components of the sensitivity of the generalized positions right after the event are given by equation (2.89)*, using the after-event constraints:*

$$Q_{\text{dep+}}|_{t_{\text{eve}}}^{+} = \mathsf{R}^{+}|_{t_{\text{eve}}}^{+} \cdot Q_{\text{dof+}}|_{t_{\text{eve}}}^{+} - \left(\Phi_{q_{\text{dep+}}}^{+}|_{t_{\text{eve}}}^{+} \right)^{-1} \Phi_{\rho}^{+} \Big|_{t_{\text{eve}}}^{+} . \tag{2.91b}$$

Proof. *The proof of the jump in the independent coordinates* (2.91a) *follows closely the proof of Theorem 2. The equation for dependent coordinates* (2.91b) *follows from the linearized* *position constraint equation* (2.89). $\square$

Remark. From (2.73) and (2.75) we can rewrite (2.91a) as:

$$\mathsf{P}^{+}_{\text{dof}+} \cdot \left(Q|^{+}_{t_{\text{eve}}} - Q|^{-}_{t_{\text{eve}}} \right) = -\mathsf{P}^{+}_{\text{dof}+} \cdot \left(v|^{+}_{t_{\text{eve}}} - v|^{-}_{t_{\text{eve}}} \right) \cdot \frac{dt_{\text{eve}}}{d\rho}. \tag{2.92}$$

2.4.4 The jump in the sensitivity of the velocity state vector

Theorem 7 (Jump in velocity sensitivity for constrained systems)**.** *Let* $V|^{+}_{t_{\text{eve}}}, V|^{-}_{t_{\text{eve}}} \in \mathbb{R}^{n\times p}$ *be the sensitivity matrices of the generalized velocity state vectors after and before the event, respectively. The independent coordinates of the velocity sensitivities right after the event are given by:*

$$\begin{aligned} V_{\text{dof}+}|^{+}_{t_{\text{eve}}} = {} & h_q|^{-}_{t_{\text{eve}}} \cdot Q|^{-}_{t_{\text{eve}}} + h_{v_{\text{dof-}}}|^{-}_{t_{\text{eve}}} \cdot V_{\text{dof-}}|^{-}_{t_{\text{eve}}} + \Big(h_q|^{-}_{t_{\text{eve}}} \cdot v|^{-}_{t_{\text{eve}}} - \ddot{q}_{\text{dof}+}|^{+}_{t_{\text{eve}}} \\ & + h_{v_{\text{dof-}}}|^{-}_{t_{\text{eve}}} \cdot \ddot{q}_{\text{dof-}}|^{-}_{t_{\text{eve}}} + h_t|^{-}_{t_{\text{eve}}} \Big) \cdot \frac{dt_{\text{eve}}}{d\rho} + h_\rho|^{-}_{t_{\text{eve}}}, \end{aligned} \tag{2.93a}$$

where the Jacobians of the jump function are:

$$\begin{aligned} & h_q|^{-}_{t_{\text{eve}}} := \frac{\partial h}{\partial q}\big(q|_{t_{\text{eve}}}, v_{\text{dof-}}|^{-}_{t_{\text{eve}}}, \rho\big) \in \mathbb{R}^{f^{+}\times n}, && h_{v_{\text{dof-}}}|^{-}_{t_{\text{eve}}} := \frac{\partial h}{\partial v_{\text{dof-}}}\big(q|_{t_{\text{eve}}}, v_{\text{dof-}}|^{-}_{t_{\text{eve}}}, \rho\big) \in \mathbb{R}^{f^{+}\times f^{-}}. \\ & h_t|^{-}_{t_{\text{eve}}} := \frac{\partial h}{\partial t}\big(q|_{t_{\text{eve}}}, v_{\text{dof-}}|^{-}_{t_{\text{eve}}}, \rho\big) \in \mathbb{R}^{f}, && h_\rho|^{-}_{t_{\text{eve}}} := \frac{\partial h}{\partial \rho}\big(q|_{t_{\text{eve}}}, v_{\text{dof-}}|^{-}_{t_{\text{eve}}}, \rho\big) \in \mathbb{R}^{f\times p}. \end{aligned} \tag{2.93b}$$

The dependent components of the velocity sensitivities right after the event are calculated via (2.90)*, using the after-event constraints:*

$$V_{\text{dep}+}\big|_{t_{\text{eve}}}^{+} = -\left(\Phi^{+}_{q_{\text{dep}+}}\big|_{t_{\text{eve}}}^{+}\right)^{-1}\left(\Phi^{+}_{q_{\text{dof}+}} \cdot V_{\text{dof}+} + \left(\Phi^{+}_{q,\,q}\,v + \Phi^{+}_{t,\,q}\right) \cdot Q + \Phi^{+}_{q,\,\rho}\,v + \Phi^{+}_{t,\,\rho}\right)\Big|_{t_{\text{eve}}}^{+} . \tag{2.93c}$$

Proof. *The proof of the jump in the independent coordinates* (2.93a) *follows closely the proof of Theorem 3. The equation for dependent coordinates* (2.93c) *follows from the linearized velocity constraint equation* (2.90)*.* □

2.4.5 The jump in the sensitivity of the velocity state vector using the hybrid DAE jump formulation

Consider the case of a sudden change in constraints discussed in Remark 2.4.2. The jump in the velocity sensitivity for constrained systems due to impulsive forces is determined as follows:

$$\begin{aligned}
&\begin{bmatrix} \mathsf{M}\big|_{t_{\text{eve}}}^{+} & {\Phi^{+}_{q}}^{\mathrm{T}}\big|_{t_{\text{eve}}}^{+} \\ \Phi^{+}_{q}\big|_{t_{\text{eve}}}^{+} & \mathsf{0} \end{bmatrix} \cdot \begin{bmatrix} V\big|_{t_{\text{eve}}}^{+} \\ \delta\Lambda \end{bmatrix} \\
&= - \begin{bmatrix} \mathsf{M}\big|_{t_{\text{eve}}\,q}^{+}\big|_{t_{\text{eve}}}^{+} \cdot \left(v\big|_{t_{\text{eve}}}^{+} - v\big|_{t_{\text{eve}}}^{-}\right) + {\Phi^{+}_{q,\,q}}^{\mathrm{T}}\big|_{t_{\text{eve}}}^{+} \cdot \delta\mu \\ \Phi^{+}_{q,\,q}\big|_{t_{\text{eve}}}^{+} \cdot v\big|_{t_{\text{eve}}}^{+} \end{bmatrix} \cdot Q\big|_{t_{\text{eve}}}^{+} + \begin{bmatrix} \mathsf{M}\big|_{t_{\text{eve}}}^{+} \\ \mathsf{0} \end{bmatrix} \cdot V\big|_{t_{\text{eve}}}^{-} \\
&\quad - \begin{bmatrix} \mathsf{M}_{\rho}\big|_{t_{\text{eve}}}^{+} \cdot v\big|_{t_{\text{eve}}}^{+} + {\Phi^{+}_{q,\,\rho}}^{\mathrm{T}}\big|_{t_{\text{eve}}}^{+} \cdot \delta\mu \\ \Phi^{+}_{q,\,\rho}\big|_{t_{\text{eve}}}^{+} \cdot v\big|_{t_{\text{eve}}}^{+} + \Phi^{+}_{t,\,q}\big|_{t_{\text{eve}}}^{+} \cdot v\big|_{t_{\text{eve}}}^{-} + \Phi^{+}_{t,\,v}\big|_{t_{\text{eve}}}^{+} \cdot v\big|_{t_{\text{eve}}}^{-} + \Phi^{+}_{t,\,\rho}\big|_{t_{\text{eve}}}^{+} \cdot v\big|_{t_{\text{eve}}}^{-} \end{bmatrix},
\end{aligned} \tag{2.94}$$

or equivalently:

$$
\begin{aligned}
&\begin{bmatrix} V|_{t_{\mathrm{eve}}}^{+} \\ \delta\Lambda \end{bmatrix} \\
&= - \begin{bmatrix} \mathsf{M} & \Phi_{q}^{+\,\mathrm{T}} \\ \Phi_{q}^{+} & \mathsf{0} \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{M}_{q} \cdot \left(v|_{t_{\mathrm{eve}}}^{+} - v|_{t_{\mathrm{eve}}}^{-}\right) + {\Phi_{q,\,q}^{+}}^{\mathrm{T}} \cdot \delta\mu \\ \Phi_{q,\,q}^{+} \cdot v|_{t_{\mathrm{eve}}}^{+} \end{bmatrix} \cdot Q|_{t_{\mathrm{eve}}}^{+} + \begin{bmatrix} \mathsf{M} & \Phi_{q}^{+\,\mathrm{T}} \\ \Phi_{q}^{+} & \mathsf{0} \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{M} \\ \mathsf{0} \end{bmatrix} \cdot V|_{t_{\mathrm{eve}}}^{-} \\
&\quad - \begin{bmatrix} \mathsf{M} & \Phi_{q}^{+\,\mathrm{T}} \\ \Phi_{q}^{+} & \mathsf{0} \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{M}_{\rho} \cdot v|_{t_{\mathrm{eve}}}^{+} + {\Phi_{q,\,\rho}^{+}}^{\mathrm{T}} \cdot \delta\mu \\ \Phi_{q,\,\rho}^{+} \cdot v|_{t_{\mathrm{eve}}}^{+} + \Phi_{t,\,\rho}^{+} \cdot v|_{t_{\mathrm{eve}}}^{-} \end{bmatrix} - \begin{bmatrix} \mathsf{M} & \Phi_{q}^{+\,\mathrm{T}} \\ \Phi_{q}^{+} & \mathsf{0} \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{0} \\ \Phi_{t,\,q}^{+} \cdot v|_{t_{\mathrm{eve}}}^{-} + \Phi_{t,\,v}^{+} \cdot v|_{t_{\mathrm{eve}}}^{-} \end{bmatrix},
\end{aligned}
\tag{2.95}
$$

which simplifies to:

$$
\begin{bmatrix} V|_{t_{\mathrm{eve}}}^{+} \\ \delta\Lambda \end{bmatrix} = f_{q}^{\text{DAE-imp}} \cdot Q|_{t_{\mathrm{eve}}}^{+} + f_{v|_{t_{\mathrm{eve}}}^{-}}^{\text{DAE-imp}} \cdot V|_{t_{\mathrm{eve}}}^{-} + f_{\rho}^{\text{DAE-imp}} + f_{t}^{\text{DAE-imp}} \tag{2.96}
$$

2.4.6 The jump in the sensitivity of the Lagrange multipliers

Remark. When the DAE formalism is selected to model the smooth dynamics of a constrained mechanical system, the jump in the sensitivity of the Lagrange multipliers (2.54) from $\Lambda|_{t_{\mathrm{eve}}}^{-} \to \Lambda|_{t_{\mathrm{eve}}}^{+}$ at the time of event is:

$$
\Lambda_i|_{t_{\mathrm{eve}}}^{+} = \Lambda_i|_{t_{\mathrm{eve}}}^{-} + f_{q}^{\text{DAE-}\mu}|_{t_{\mathrm{eve}}}^{+}\, Q_i|_{t_{\mathrm{eve}}}^{+} + f_{v}^{\text{DAE-}\mu}|_{t_{\mathrm{eve}}}^{+}\, V_i|_{t_{\mathrm{eve}}}^{+} + f_{\rho_i}^{\text{DAE-}\mu}|_{t_{\mathrm{eve}}}^{+}, \quad i = 1, \ldots, p \tag{2.97}
$$

Remark. When the ODE penalty formalism is selected to model the smooth dynamics of a constrained mechanical system, the jump in the sensitivity of the estimated Lagrange multipliers (2.71) from $\Lambda^*|_{t_{\rm eve}}^- \to \Lambda^*|_{t_{\rm eve}}^+$ at the time of event is:

$$\Lambda_i^*|_{t_{\rm eve}}^+ = \Lambda_i^*|_{t_{\rm eve}}^- + \mu_q^*|_{t_{\rm eve}}^+ \, Q_i|_{t_{\rm eve}}^+ + \mu_v^*|_{t_{\rm eve}}^+ \, V_i|_{t_{\rm eve}}^+ + \mu_{\rho_i}^*|_{t_{\rm eve}}^+, \quad i = 1, \dots, p \tag{2.98}$$

2.4.7 The sensitivity of the cost function for hybrid systems

Remark. The formalism that computes the sensitivities of the cost function with respect to parameters for hybrid systems does not change from the formalism presented for smooth systems illustrated in Remark 2.1.3. Indeed, the sensitivities of the cost function sum all the sensitivities of the trajectories and the quadrature variables evaluated at the final time. Any jump in the sensitivities of the trajectories and quadrature variables were anteriorly computed. The jump in the sensitivities of the quadrature variables are given by (2.49).

2.5 Direct sensitivity analysis for constrained mechanical systems with transition functions

The transition function refers to a sudden change of the governing function or vector field. In this section we discuss about direct sensitivity analysis for constrained mechanical with jump-discontinuity in the acceleration caused by a sudden change of the equation of motions at the time of event.

Definition 2.5.1 (Change of EOM at the time of event)**.** Unlike previous methodology, the ODE penalty formulation (2.66) incorporates the kinematic constraints (position, velocity, and acceleration constraint equations) into the equation of motions and stabilize them over time. Therefore, any change in the set of kinematic constraints involves a change in the equation of motions, thus, a change in the acceleration vector (or right-hand side function). Because the ODE penalty formulation is a control based constraint stabilization method, the position constraint is not satisfied exactly right after the sudden change in the set of kinematic constraints:

$$\Phi^{-}|_{t_{\text{eve}}}^{-} = 0, \quad \Phi^{+}|_{t_{\text{eve}}}^{+} \neq 0. \tag{2.99}$$

This differs from (2.85) as there are no instantaneous kinematic jump in the velocity state variable.

Theorem 8 (Jump in the velocity sensitivity for constrained systems due to the change of equation of motions)**.** *Let* $V|_{t_{\text{eve}}}^{+}, V|_{t_{\text{eve}}}^{-} \in \mathbb{R}^{n \times p}$ *be the sensitivity matrices of the generalized velocity state vectors after and before the event, respectively. Let the event characterized as a change of equation of motions due to the change of constraints including in the equation of motions. The sensitivities of the independent velocities right after the event are given by*

$$V_{\text{dof-}}|_{t_{\text{eve}}}^{+} = V_{\text{dof-}}|_{t_{\text{eve}}}^{-} + \left(\ddot{q}_{\text{dof-}}|_{t_{\text{eve}}}^{-} - \ddot{q}_{\text{dof-}}|_{t_{\text{eve}}}^{+}\right) \cdot \frac{dt_{\text{eve}}}{d\rho}. \tag{2.100}$$

Proof. The proof of the jump in the independent coordinates (58a) follows closely the proof of Theorem 4. □

Remark. The sensitivities of the dependent velocities right after the event are given by (2.93c). As well, the sensitivities of the position right after the event for the independent and dependent variables are given by (2.91a) and (2.91b), respectively.

Remark. The sudden change in the equation of motions at the event time is caused by a sudden change of forces acting on the system, such as constraint forces, friction forces, or a change of masses. The proposed formalism to calculate the jump conditions for systems with discontinuous right-hand sides remains valid for any type of change of the equation of motions.

Remark. The proposed formalism in calculating the jump conditions for systems with jerk discontinuity incorporates Remarks 2.4.6 and 2.4.7.

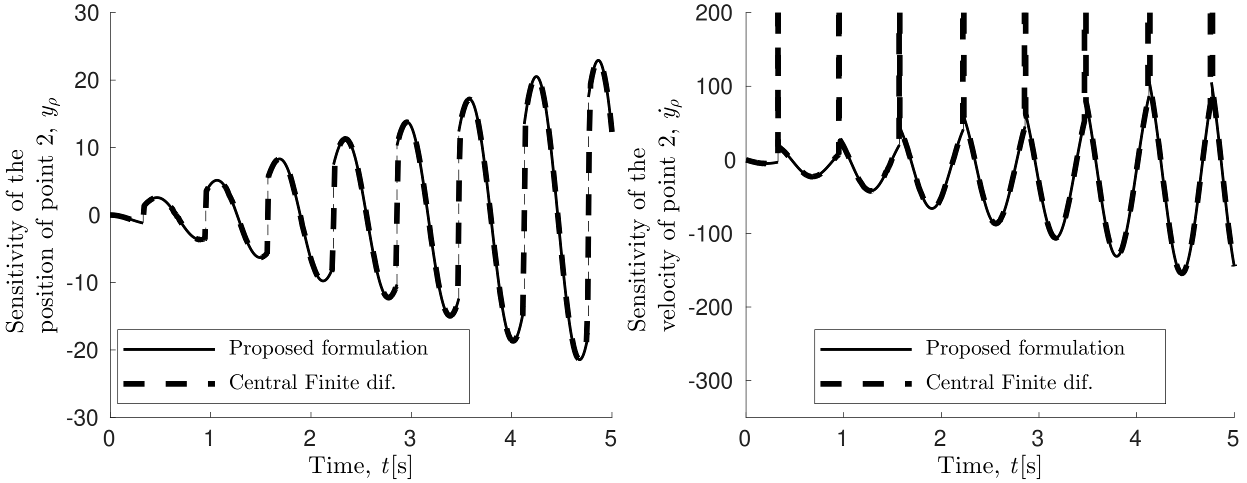
2.6 Case study: sensitivity analysis of a five-bar mechanism

A five-bar mechanism is used as a case study to apply the presented mathematical framework. The presentation of the mechanism and the evolution of the position and velocity trajectories of the bottom point of the mechanism are provided in Appendix C.

The trajectories of the sensitivity of the position and velocity of point 2 of the five-bar mechanism along the vertical y axis are shown in Fig. 2.3a and Fig. 2.3b, respectively.

The jump equations of the sensitivity of the position and velocity at each time of event were determined from (2.91) and (7), respectively. The results of the analytical sensitivity presented in this paper is benchmarked against the central finite difference, which consists on differentiating the trajectories of the position and velocity of point 2 for a perturbed system on the parameters $\delta\rho$ with the nominal trajectories computed from the initial system. The difference is then divided by $\delta\rho$. We refer the central finite difference methodology as a numerical sensitivity analysis.

The analytical sensitivity is represented by the continuous line, while the central finite difference sensitivity is represented by the dashed line. There is an excellent correlation between the numerical and the analytical sensitivities, with a difference between the two trajectories of less than 0.1%. Note that the numerical sensitivity of the velocity of point 2 along the vertical axis tends to be really large in magnitude, $1/\delta\rho$ at each time of event. This is shown by the vertical dashed lines and it is due to the fact that the difference between the trajectories $v(\rho+\delta\rho)$ and $v(\rho-\delta\rho)$ increases considerably during the Δt period, as shown in Fig. 2.2. Indeed, the magnitude of the difference of the trajectories $|v(\rho+\delta\rho)|^{+}_{t_{\text{eve}}} - v(\rho-\delta\rho)|^{-}_{t_{\text{eve}}}| = |h(v(\rho+\delta\rho)|^{-}_{t_{\text{eve}}}) - v(\rho-\delta\rho)|^{-}_{t_{\text{eve}}}| = |-v(\rho+\delta\rho)|^{-}_{t_{\text{eve}}} - v(\rho-\delta\rho)|^{-}_{t_{\text{eve}}}| \approx |-2\,v(\rho-\delta\rho)|^{-}_{t_{\text{eve}}}|$. This difference divided by $\delta\rho$ of magnitude 10^{-4} leads the jump in the numerical sensitivity of the velocity of point 2 to 10^{4} of magnitude. Therefore, this result shows that the novel analytical sensitivity method presented in this paper is considerably more robust than the numerical method, as it correctly calculates the sensitivity jumps and accurately determines the sensitivity trajectories after each event without any delta-like jumps.

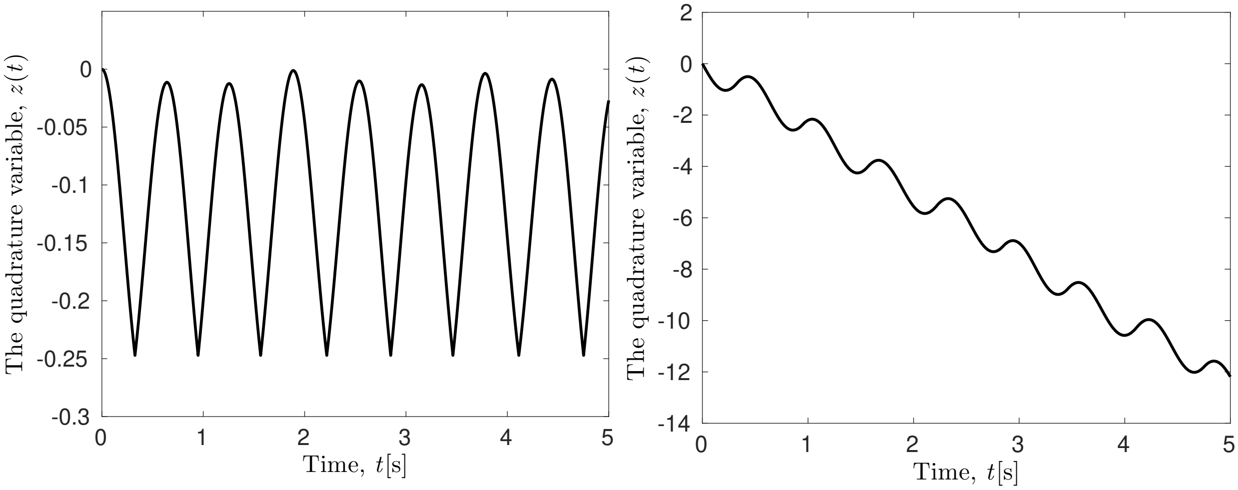


(a) The sensitivity of the position of the bottom point y_2 of the five-bar mechanism

(b) The sensitivity of the velocity of the bottom point $\dot{y}_2$ of the five-bar mechanism

Figure 2.3: Sensitivity analysis of the position and velocity of the bottom point of the five-bar mechanism

The trajectories of the quadrature variables $z(t) = \int_{t_0}^{t} \dot{y}_2(\tau)\ \mathrm{d}\tau$ and $z(t) = \int_{t_0}^{t} \ddot{y}_2(\tau)\ \mathrm{d}\tau$ are shown in Fig. 2.4a and Fig. 2.4b, respectively. Note that $z(t) = \int_{t_0}^{t} \dot{y}_2(\tau)\ \mathrm{d}\tau$ matches the trajectory of the position of point 2 along the vertical axis in Fig. C.2a, while $z(t) = \int_{t_0}^{t} \ddot{y}_2(\tau)\ \mathrm{d}\tau$ does not completely match the trajectory of the velocity of point 2 in Fig. C.2b. This is due to the fact that the velocity variable is affected by the impulse function at the time of event, while the quadrature variable is not. The trajectories after each event differ by a constant since the quadrature variable evaluates the integral of the acceleration of point 2.

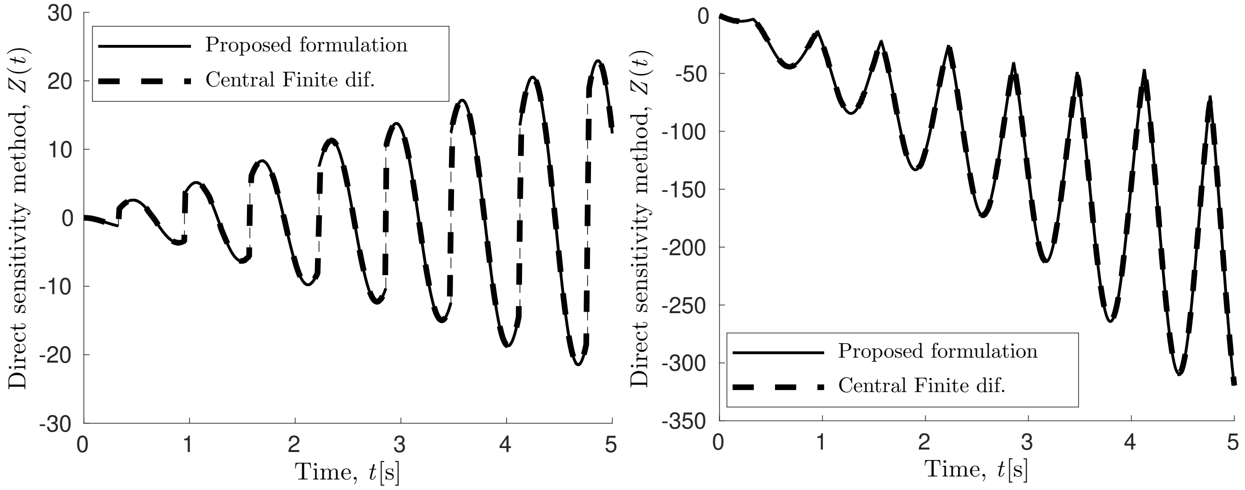


(a) The quadrature variable $z(t) = \int_{t_0}^{t} \dot{y}_2(\tau)\ \mathrm{d}\tau$

(b) The quadrature variable $z(t) = \int_{t_0}^{t} \ddot{y}_2(\tau)\ \mathrm{d}\tau$

Figure 2.4: The quadrature variables of the five-bar mechanism.

The trajectories of the sensitivities of the quadrature variables $z(t) = \int_{t_0}^{t} \dot{y}_2(\tau)\ \mathrm{d}\tau$ and $z(t) = \int_{t_0}^{t} \ddot{y}_2(\tau)\ \mathrm{d}\tau$ are presented in Fig. 2.5a and Fig. 2.5b, respectively. The sensitivities are with respect to the system parameters $\rho = \begin{bmatrix} L_{01} & L_{02} \end{bmatrix}$. The results of the analytical and numerical sensitivity analysis of the five-bar mechanism highlight the quasi-perfect correlation between the numerical and analytical sensitivities with a difference between the two trajectories of less than 0.1%. Note that a similar observation with the one previously made is valid here: the sensitivity of $z(t) = \int_{t_0}^{t} \dot{y}_2(\tau)\ \mathrm{d}\tau$ shown in Fig. 2.5a matches the trajectory of the sensitivity of the position illustrated in Fig. 2.3a, while the sensitivity of $z(t) = \int_{t_0}^{t} \ddot{y}_2(\tau)\ \mathrm{d}\tau$ shown in Fig. 2.5b does not completely match the trajectory of the sensitivity of the velocity from Fig. 2.3b because of the impulse function.



(a) The sensitivity of $z(t) = \int_{t_0}^{t} \dot{y}_2(\tau)\, \mathrm{d}\tau$ with $Z = \frac{dz}{d\rho}$.

(b) The sensitivity of $z(t) = \int_{t_0}^{t} \ddot{y}_2(\tau)\, \mathrm{d}\tau$ with $Z = \frac{dz}{d\rho}$

Figure 2.5: Sensitivity analysis of the quadrature variables of the five-bar mechanism

2.7 Case study: sensitivity analysis of the Iltis vehicle

The mathematical framework is now applied to the Iltis vehicle Fig. 2.6. This vehicle is a commonly used as a benchmark problem by the European automobile industry for multibody dynamic simulation. The optimization of this vehicle under different scenaries (four-post test, handling, syhmpeed bumps test, vehicle handling) was presented in [1, 2].

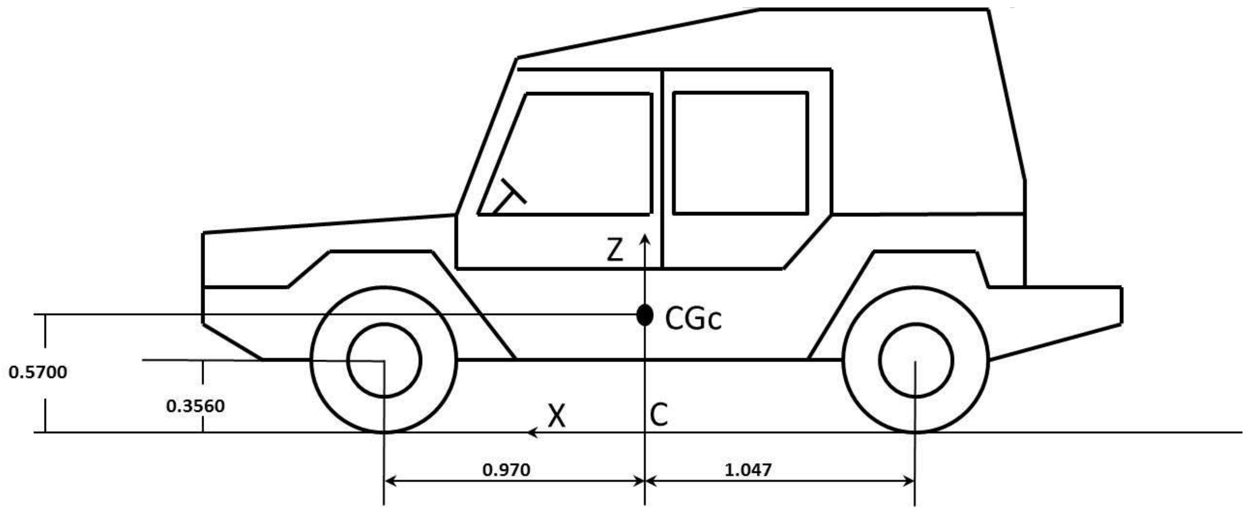


Figure 2.6: Diagram of the Iltis vehicle.

The topology of the vehicle is presented in the diagram Fig. 2.7. The vehicle is composed of twenty bodies that mainly include the chassis, four identical suspension systems linked to each wheel, a tie and a steering rod. The system is linked by sixteen revolute and eight spherical joints. In this example, only the vertical motion of the vehicle is considered, thus, the steering system was removed for simplicity. More details on the numerical values of the parameters are provided in [1].

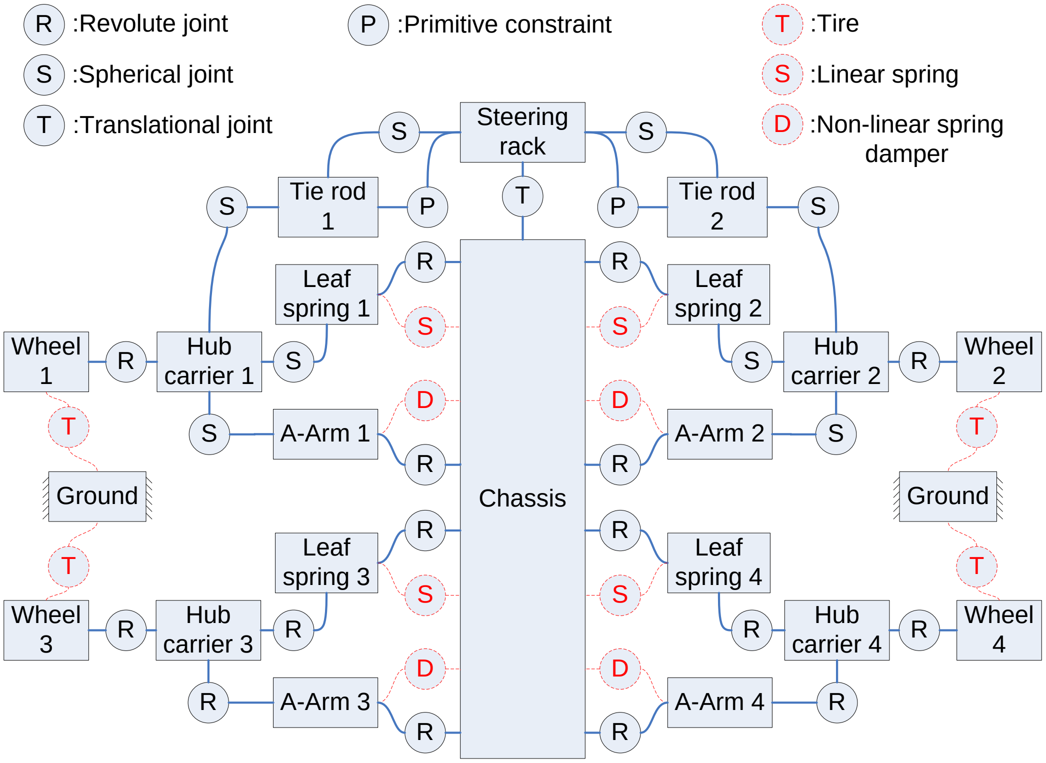


Figure 2.7: Topology of the Iltis vehicle.

The study consists of dropping the vehicle 0.5 m and let it settle for two seconds. Normal forces are applied on the wheels using the Kelvin-Voigt model [1]. The vertical position of the center of gravity (CG) of the vehicle is shown in Fig. 2.8. The ground level is located at zero. The wheels are in contact with the ground at around 0.4s. Note that the damping coefficients of the suspensions were lowered to $1000N/m$ allowing the system to oscillate. Then, an event $q_{chassis} - 0.6 = 0$ was added and only enabled when $t > 2sec$. As seen in the plot, the event is triggered around $t_{eve} = 2, 1s$. The values of the position of the chassis right before and after the time of the event are displayed by circle markers.

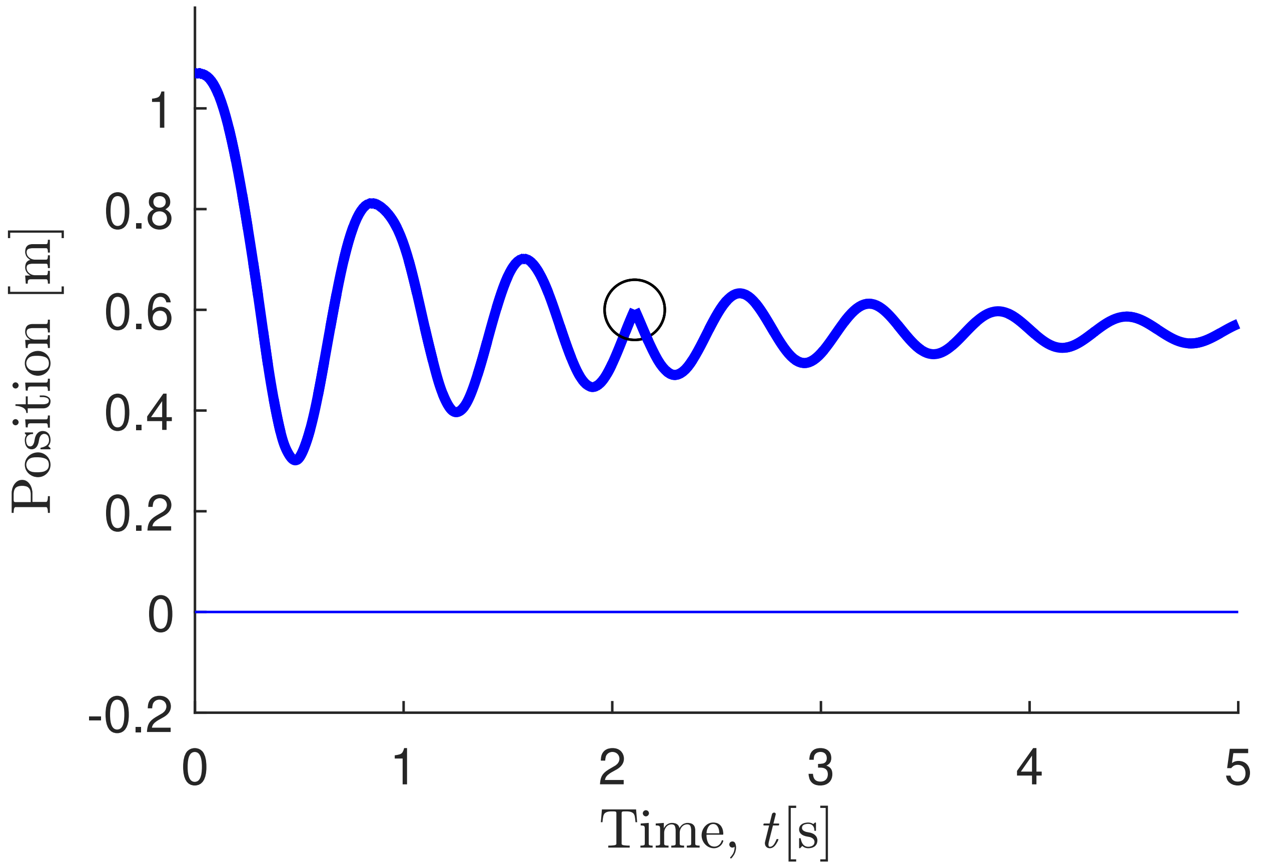


Figure 2.8: The vertical position of the Iltis vehicle, the circle marker displays the value of the position at the event, the position of the vehicle remains the same.

The velocity of the vehicle is shown in Fig. 2.9. We set the jump equation at the event such as the vertical velocity of the chassis suddenly jumps to its opposite value. The values of the vertical velocity before and after the time of the event are shown by circle markers.

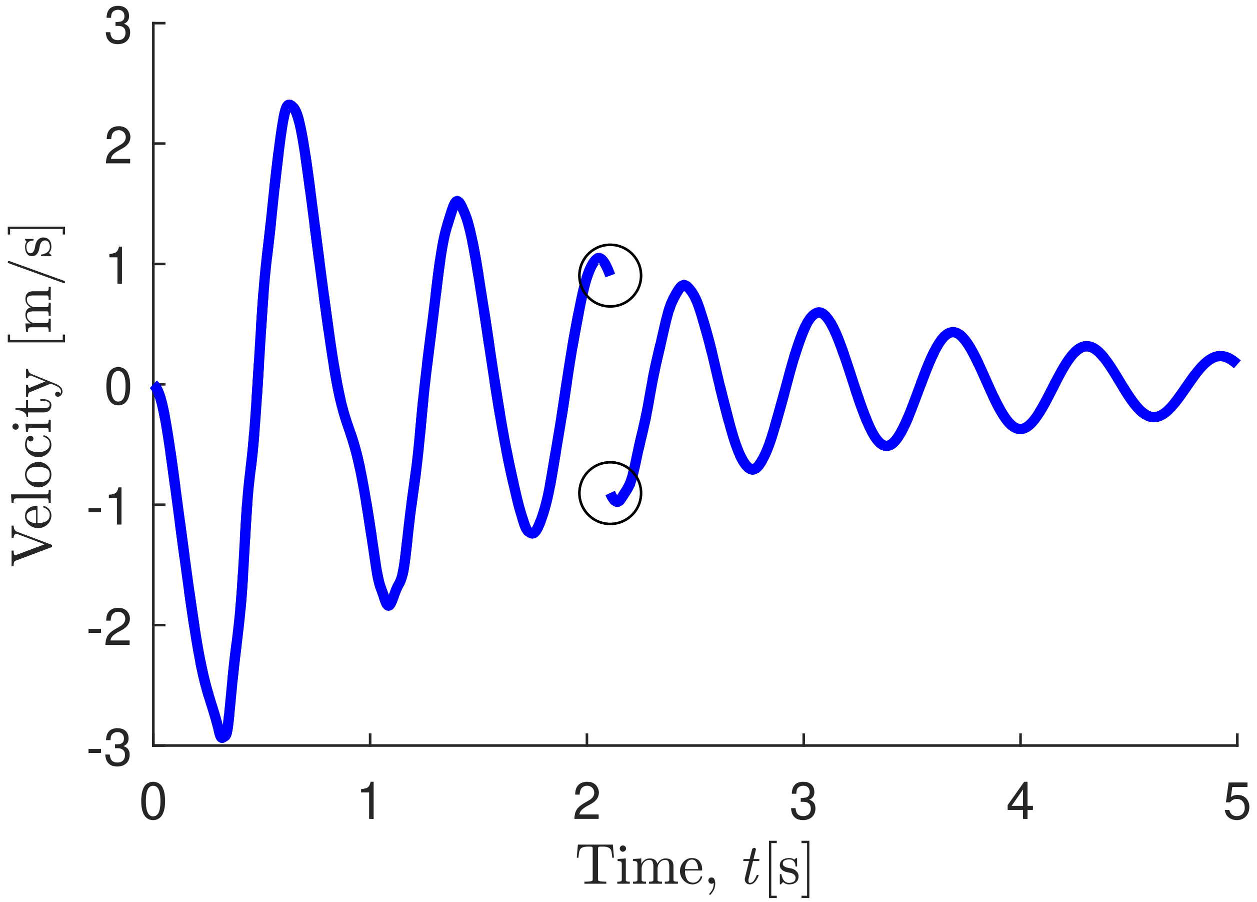


Figure 2.9: The vertical velocity of the Iltis vehicle, the circle marker displays the value of the velocity at the event, jumping from its velocity value before event to its opposite sign after event.

The sensitivity of the vertical position and velocity of the CG of the chassis with respect to the initial length of the right rear leaf spring are presented in Fig. 2.10 and Fig. 2.11. The proposed formulation is benchmarked with the central finite difference with a perturbation $\delta = 10^{-4}$. The solution of the proposed method and the finite difference are drawn with the red and blue lines, respectively. It is observed that the finite difference results become really noisy after the vehicle impacts the ground at around 0.4s, while the proposed formulation keeps the trajectory of the sensitivities smooth. The proposed formulation jumps the sensitivities right after the time of the event close to the the values of the finite difference.

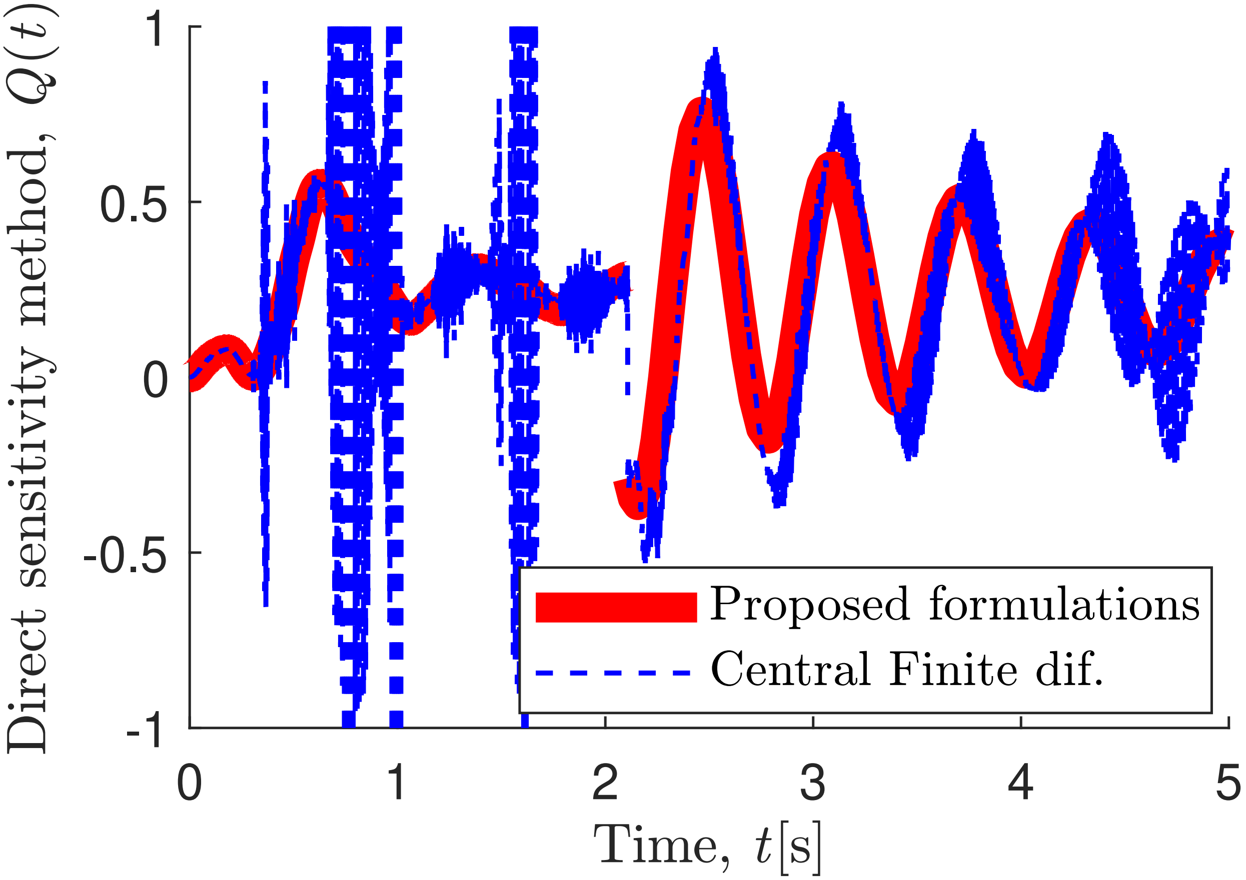


Figure 2.10: The sensitivity $Q_{chassis}$ of the vertical position of the Iltis vehicle $q_{chassis}$ with respect to the initial length of right rear leaf spring.

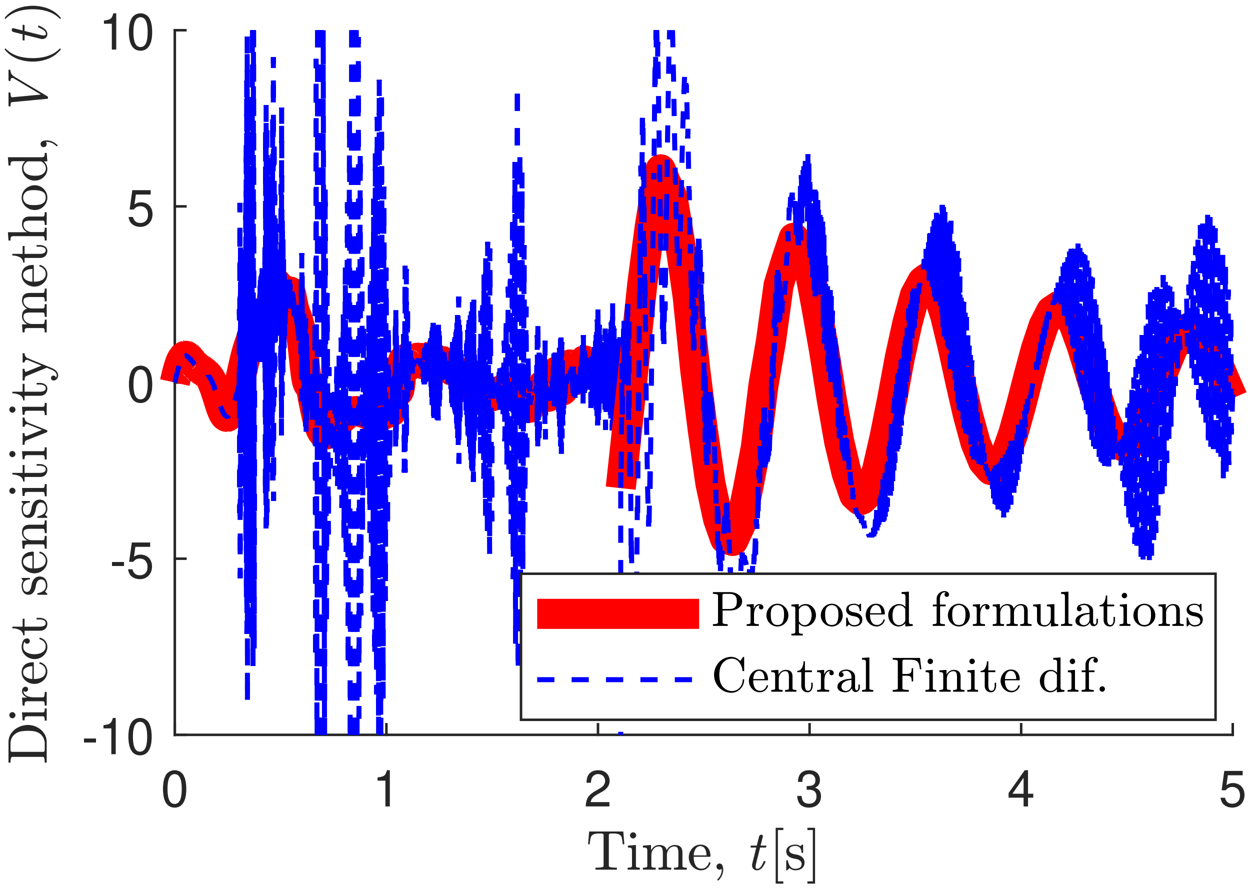


Figure 2.11: The sensitivity $V_{chassis}$ of the vertical velocity of the Iltis vehicle $v_{chassis}$ with respect to the initial length of right rear leaf spring.

Note that the finite difference is really sensitive to the integration method and its relative and absolute tolerances. An Explicit Runge-Kutta integrator with an event detection algorithm was used. A slight changes in the tolerances changed the finite difference results considerably as shown in Fig. 2.12 and Fig. 2.13.

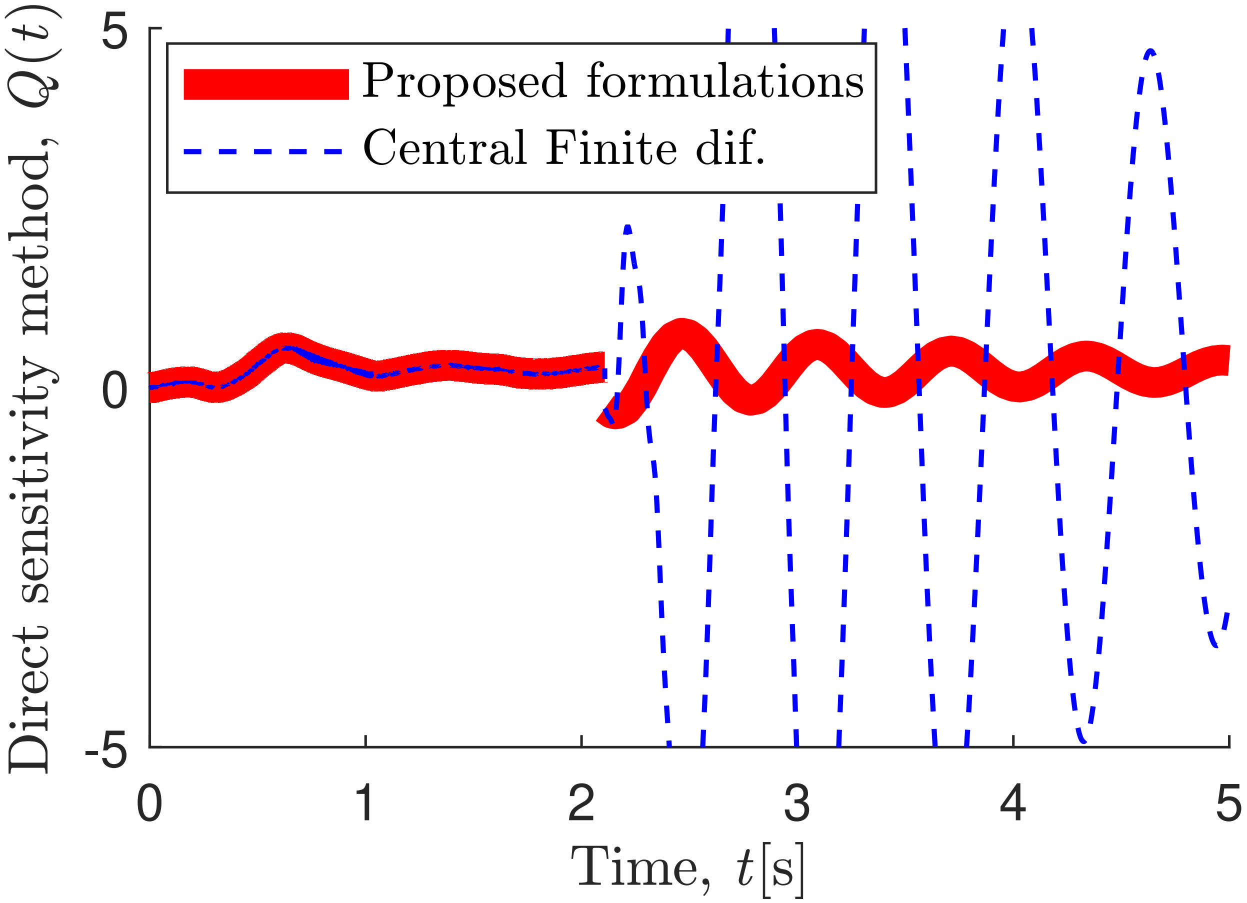


Figure 2.12: The sensitivity $Q_{chassis}$ of the vertical position of the Iltis vehicle $q_{chassis}$ with respect to the initial length of right rear leaf spring.

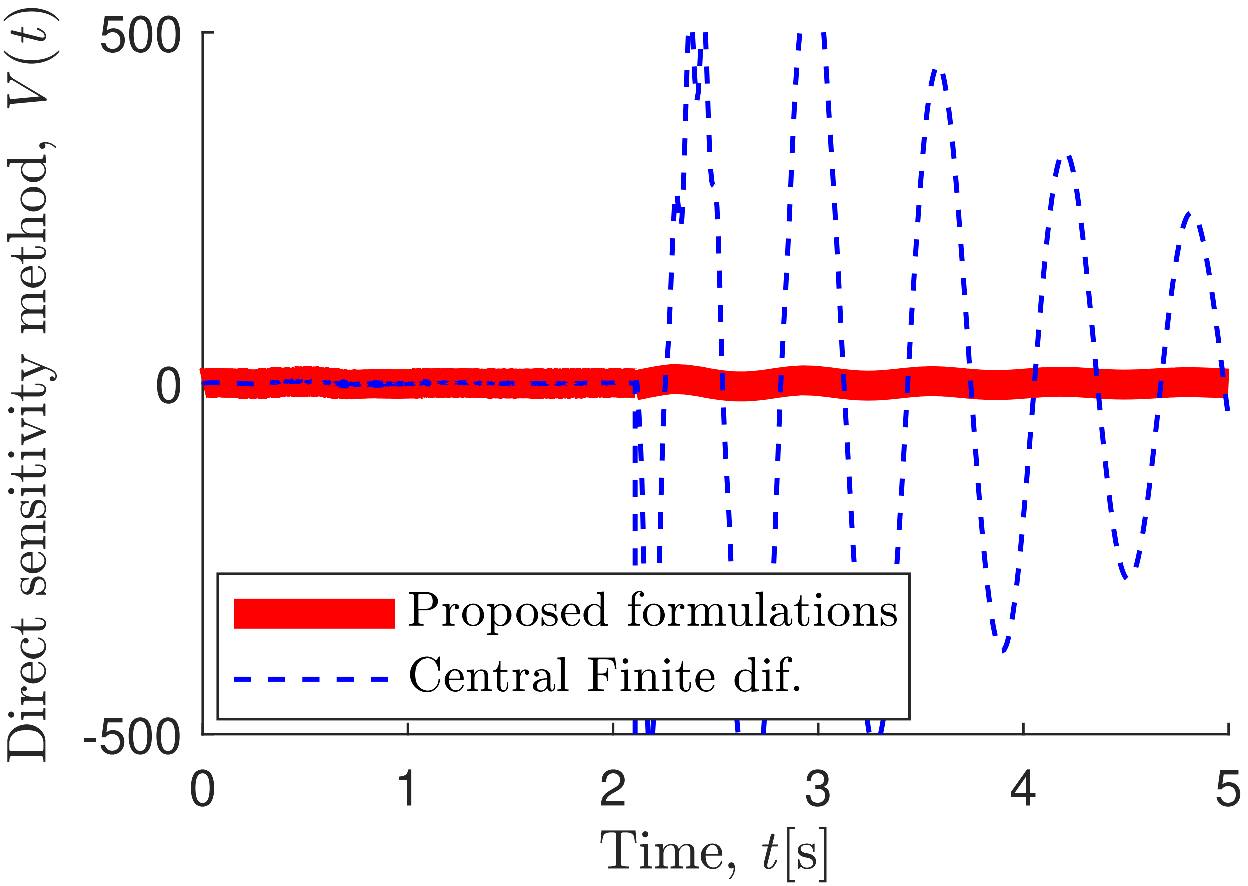


Figure 2.13: The sensitivity $V_{chassis}$ of the vertical velocity of the Iltis vehicle $v_{chassis}$ with respect to the initial length of right rear leaf spring.

Therefore, this case study clearly shows the necessary used of an analytically analysis when solving the sensitivities of complex multibody systems. The finite difference cannot be trustful if the mechanical system has forward non-smooth trajectories.

It is also noted that the kinematic constraints should be rectified using a Newton algorithm. Indeed, the penalty methods accumulate errors in the kinematics that may lead the jump equations to be inaccurate and the forward trajectories after the event to diverge from its true solution. The forward trajectories after the event should be continuous under the Lipschitz conditions, meaning the initial conditions of those trajectories should be really close to the true values [63].

Chapter 3

Modeling and Adjoint Sensitivity Analysis Methodology

3.1 Sensitivity analysis for unconstrained mechanical systems and extended cost functions

This section implement the direct and adjoint sensitivity analysis for dynamical systems governed by smooth second order systems of ordinary differential equations (2nd order ODEs). This method is extended to n_c cost functions that contain argument function and the sensitivity analysis is with respect to n_p parameters.

3.1.1 Smooth ODE systems dynamics and extended cost functions

We consider an unconstrained mechanical system governed by the second order ordinary differential equation (ODE):

$$\begin{aligned} \mathsf{M}\left(t, q, \rho\right) \cdot \ddot{q} = \mathsf{F}\left(t, q, \dot{q}, \rho\right), \quad t_0 \leq t \leq t_F, \quad q(t_0) = q_0(\rho), \quad \dot{q}(t_0) = \dot{q}_0(\rho), \\ \Leftrightarrow \quad \ddot{q} = \mathsf{M}^{-1}\left(t, q, \rho\right) \cdot \mathsf{F}\left(t, q, \dot{q}, \rho\right) =: f^{\mathrm{eom}}\left(t, q, \dot{q}, \rho\right), \end{aligned} \tag{3.1}$$

where $q \in \mathbb{R}^n$ are the generalized positions, $v := \dot{q} \in \mathbb{R}^n$ the generalized velocities, and $\rho \in \mathbb{R}^p$ the time independent parameters of the system. The state trajectories depend implicitly on time and on the parameters, $q = q(t, \rho)$ and $v = \dot{q}(t, \rho)$. We consider a general system output of the form:

$$\psi(\rho) = \int_{t_0}^{t_F} \tilde{g}_j\big(t, q, v, \rho\big)\, dt + \tilde{w}\big(t_F, q_{t_F}, v_{t_F}, \rho\big), \quad q_{t_F} := q(t_F, \rho), \quad v_{t_F} := v(t_F, \rho). \tag{3.2}$$

The function $\tilde{g} : \mathbb{R}^{1+2n+p} \to \mathbb{R}^{n_c}\wr$ is a vector of 'trajectory cost functions', and $\tilde{w} : \mathbb{R}^{1+2n+p} \to \mathbb{R}^{n_c}$ is a vector of 'terminal cost functions', and the system output $\psi \in \mathbb{R}^{n_c}$ is a vector of n_c 'outputs', i.e., scalar cost functions. Both the trajectory and terminal cost functions can include accelerations via $\dot{v}$. Accelerations are not independent variables and can be resolved in terms of positions and velocities $\dot{v} := f^{\mathrm{eom}}\left(t, q, \dot{q}, \rho\right) \in \mathbb{R}^n$. The cost functions can also include arguments $\tilde{u}\big(\,t,\, q,\, v,\, \rho\,\big) = u\left(\,t,\, q,\, v,\, \dot{v},\, \rho\right)$ that depend on the solution and on the acceleration. Our notation encompasses these cases by defining:

$$\begin{aligned} \tilde{g}\big(\, t,\, q,\, v,\, \rho \,\big) &= g\big(\, t,\, q,\, v,\, \dot{v},\, \rho,\, u(\, t,\, q,\, v,\, \dot{v}, \rho)\big), \\ \tilde{w}\big(t_F, q_{t_F}, v_{t_F}, \rho\big) &= w\left(t_F, q_{t_F}, v_{t_F}, \dot{v}_{t_F}, \rho, u(t_F, q_{t_F}, v_{t_F}, \dot{v}_{t_F}, \rho)\right). \end{aligned} \tag{3.3}$$

All functions are considered to be smooth.

Definition 3.1.1 (Sensitivity analysis problem)**.** The sensitivity analysis problem is to compute the derivatives of the model outputs (3.2) with respect to model parameters:

$$\frac{d\,\psi}{d\,\rho} := \left[\frac{d\,\psi}{d\,\rho_1} \cdots \frac{d\,\psi}{d\,\rho_p}\right] \in \mathbb{R}^{n_c \times p}. \tag{3.4}$$

Definition 3.1.2 (The canonical ODE system)**.** To simplify the representation of the system we define the vector of 'quadrature' variables $z \in \mathbb{R}^{n_c}$ as follows:

$$\begin{aligned} & z(t,\rho) := \int_{t_0}^{t} \tilde{g}\big(\tau, q, v, \rho\big)\, d\tau \quad \Leftrightarrow \\ & \dot{z}(t,\rho) = \tilde{g}\big(t, q, v, \rho\big), \quad t_0 \le t \le t_F, \quad z(t_0,\rho) = 0, \end{aligned} \tag{3.5}$$

which leads the vector of cost function (3.2) at final time to become:

$$\psi = z(t_F) + \tilde{w}\big(t_F, q_{t_F}, v_{t_F}, \rho\big). \tag{3.6}$$

Next, we add dummy evolution equations $\rho' = 0$ for the time independent parameters.

Finally, we append the parameters and the quadrature variables to system state to obtain the following extended ‘canonical’ state vector:

$$x(t) := \begin{bmatrix} q(t)^T & v(t)^T & \rho(t)^T & z(t)^T \end{bmatrix}^T \in \mathbb{R}^{(2n+p+n_c)\times 1}$$

together with the ‘canonical ODE system’ that describes its evolution:

$$\dot{x} = \begin{bmatrix} v \\ f^{\text{eom}}\big(t, q, v, \rho\big) \\ \mathsf{0}_{p\times 1} \\ \tilde{g}(\,t,\, q,\, v,\, \rho\,) \end{bmatrix} := F(t, x, \rho) \in \mathbb{R}^{2n+p+n_c}, \quad t_0 \le t \le t_F, \quad x(t_0) := \begin{bmatrix} q_0(\rho) \\ v_0(\rho) \\ \rho \\ \mathsf{0}_{n_c\times 1} \end{bmatrix}. \tag{3.7}$$

3.1.2 Direct sensitivity analysis for smooth ODE systems and extended cost function

Define the ‘position sensitivity’ matrix $Q(t,\rho)$, the ‘velocity sensitivity’ matrix $V(t,\rho)$, the ‘quadrature sensitivity’ matrix $Z(t,\rho)$, and an identity matrix Γ as the formal sensitivity of the parameters, as:

$$Q_i(t,\rho) := \frac{d\,q(t,\rho)}{d\,\rho_i} \in \mathbb{R}^n, \quad i = 1,\dots,p; \quad Q(t,\rho) := \begin{bmatrix} Q_1(t,\rho) \cdots Q_p(t,\rho) \end{bmatrix} \in \mathbb{R}^{n\times p}, \tag{3.8a}$$

$$V_i(t,\rho) := \frac{d\,v(t,\rho)}{d\,\rho_i} \in \mathbb{R}^n, \quad i = 1,\dots,p; \quad V(t,\rho) := \begin{bmatrix} V_1(t,\rho) \cdots V_p(t,\rho) \end{bmatrix} \in \mathbb{R}^{n\times p}, \tag{3.8b}$$

$$\Gamma_i(t,\rho) := \frac{d\,\rho(t,\rho)}{d\,\rho_i} \in \mathbb{R}^p, \quad i = 1,\dots,p; \quad \Gamma(t,\rho) := \begin{bmatrix} \Gamma_1 & \cdots & \Gamma_p \end{bmatrix} = \mathsf{I}_{p\times p}, \tag{3.8c}$$

$$Z_i(t,\rho) := \frac{\partial z(t,\rho)}{\partial \rho_i} \in \mathbb{R}^{n_c}, \quad i = 1,\dots,p; \quad Z(t,\rho) := \begin{bmatrix} Z_1(t,\rho) \cdots Z_p(t,\rho) \end{bmatrix} \in \mathbb{R}^{n_c\times p}. \tag{3.8d}$$

The direct sensitivity for ODE systems, referred to as the Tangent Linear Model (TLM), computes the sensitivity matrix $X = \left[Q^{\mathrm{T}},\, V^{\mathrm{T}},\, \Gamma,\, Z^{\mathrm{T}}\right]^{\mathrm{T}} \in \mathbb{R}^{(2n+p+n_c)\times p}$. obtained by differentiating the canonical ODE system (3.7) with respect to the parameters:

$$\dot{X} = \begin{bmatrix} \dot{Q} \\ \dot{V} \\ \dot{\Gamma} \\ \dot{Z} \end{bmatrix} = \begin{bmatrix} V \\ f_q^{\mathrm{eom}} Q + f_v^{\mathrm{eom}} V + f_\rho^{\mathrm{eom}} \\ \mathsf{0}_{p\times p} \\ \tilde{g}_q\, Q + \tilde{g}_v\, V + \tilde{g}_\rho \end{bmatrix}, \quad t_0 \le t \le t_F, \quad X(t_0) := \begin{bmatrix} \dfrac{dq_0(\rho)}{d\rho} \\ \dfrac{dv_0(\rho)}{d\rho} \\ \mathsf{I}_{p\times p} \\ \mathsf{0}_{n_c\times p} \end{bmatrix} \in \mathbb{R}^{(2n+p+n_c)\times p} \tag{3.9}$$

The direct sensitivity for ODE systems needs to be solved forward in time. The expressions f_q^{eom}, f_v^{eom}, and $f_{\rho_i}^{\mathrm{eom}}$ denote the partial derivatives of f^{eom} with respect to the subscripted variables. The detailed calculation of these expressions and the remaining partial derivatives is explained in Appendix B. Once the sensitivities (3.9) have been calculated, the sensitivities of the cost functions (3.4) with respect to parameters are computed as follows:

$$\frac{d\,\psi}{d\,\rho} = Z(t_F) + \left[\tilde{w}_q \cdot Q + \tilde{w}_v \cdot V + \tilde{w}_\rho\right]_{t_F} \in \mathbb{R}^{n_c\times p}. \tag{3.10}$$

We note that the TLM system (3.9) can be written in matrix form as follows:

$$\begin{bmatrix} \dot{Q} \\ \dot{V} \\ \dot{\Gamma} \\ \dot{Z} \end{bmatrix} = \begin{bmatrix} \mathsf{0}_{n\times n} & \mathrm{I}_{n\times n} & \mathsf{0}_{n\times p} & \mathsf{0}_{n\times n_c} \\ f_q^{\mathrm{eom}} & f_v^{\mathrm{eom}} & f_\rho^{\mathrm{eom}} & \mathsf{0}_{n\times n_c} \\ \mathsf{0}_{p\times n} & \mathsf{0}_{p\times n} & \mathsf{0}_{p\times p} & \mathsf{0}_{p\times n_c} \\ \tilde{g}_q & \tilde{g}_v & \tilde{g}_\rho & \mathsf{0}_{n_c\times n_c} \end{bmatrix} \cdot \begin{bmatrix} Q \\ V \\ \Gamma \\ Z \end{bmatrix}, \quad t_0 \le t \le t_F. \tag{3.11}$$

3.1.3 Adjoint sensitivity analysis for smooth ODE systems and extended cost function

In this section we provide the system of equations that governs the adjoint sensitivity analysis for smooth ODE systems.

Definition 3.1.3 (Adjoint sensitivity analysis)**.** Apply the chain rule differentiation to the total sensitivity of the cost function (3.4):

$$\frac{d\,\psi}{d\,\rho} = \frac{d\,\psi}{d\,x(t,\rho)} \cdot \frac{d\,x(t,\rho)}{d\,\rho} = \lambda^{\mathrm{T}}(t,\rho) \cdot X(t,\rho), \tag{3.12}$$

where $\lambda = (d\,\psi/d\,x)^T = \left[\lambda^{Q^{\mathrm{T}}}, \lambda^{V^{\mathrm{T}}}, \lambda^{\Gamma^{\mathrm{T}}}, \lambda^{Z^{\mathrm{T}}}\right]^{\mathrm{T}}$ is defined as:

$$\begin{aligned}
\lambda_j^Q(t,\rho) &:= \left(\tfrac{d\,\psi_j}{d\,q(t,\rho)}\right)^T \in \mathbb{R}^{n\times 1},\ \ j=1,\dots,n_c; & \lambda^Q(t,\rho) &:= \left[\lambda_1^Q(t,\rho)\cdots\lambda_{n_c}^Q(t,\rho)\right] \in \mathbb{R}^{n\times n_c}, && (3.13)\\
\lambda_j^V(t,\rho) &:= \left(\tfrac{d\,\psi_j}{d\,v(t,\rho)}\right)^T \in \mathbb{R}^{n\times 1},\ \ j=1,\dots,n_c; & \lambda^V(t,\rho) &:= \left[\lambda_1^V(t,\rho)\cdots\lambda_{n_c}^V(t,\rho)\right] \in \mathbb{R}^{n\times n_c}, && (3.14)\\
\lambda_j^\Gamma(t,\rho) &:= \left(\tfrac{d\,\psi_j}{d\,\rho}\right)^T \in \mathbb{R}^{p\times 1},\ \ j=1,\dots,n_c; & \lambda^\Gamma(t,\rho) &:= \left[\lambda_1^\Gamma(t,\rho)\cdots\lambda_{n_c}^\Gamma(t,\rho)\right] \in \mathbb{R}^{p\times n_c}, && (3.15)\\
\lambda_j^Z(t,\rho) &:= \left(\tfrac{d\,\psi_j}{d\,z(t,\rho)}\right)^T \in \mathbb{R}^{n_c\times 1},\ \ j=1,\dots,n_c; & \lambda^Z(t,\rho) &:= \left[\lambda_1^Z \quad \dots \quad \lambda_{n_c}^Z\right] \in \mathsf{I}_{n_c\times n_c}. && (3.16)
\end{aligned}$$

Note that, from (3.5)–(3.6)

$$\psi = z(t,\rho) + \int_\tau^{t_F} \tilde{g}\big(\tau,q,v,\rho\big)\,d\tau + \tilde{w}\big(t_F, q_{t_F}\big),$$

which leads to the relation $d\psi/dz(t,\rho) = \mathsf{I}_{n_c\times n_c}$ for any time t.

From (3.12) we have that for any time t:

$$\frac{d\,\psi}{d\,\rho} = \lambda^{Q}(t,\rho)^{\mathrm{T}} \cdot Q(t,\rho) + \lambda^{V}(t,\rho)^{\mathrm{T}} \cdot V(t,\rho) + \lambda^{\Gamma}(t,\rho)^{\mathrm{T}} + \lambda^{Z}(t,\rho)^{\mathrm{T}} \cdot Z(t,\rho). \tag{3.17}$$

Evaluating (3.17) at $t = t_F$ leads to the direct sensitivity approach:

$$\frac{d\,\psi}{d\,\rho} = \lambda^{Q}(t_F,\rho)^{\mathrm{T}} \cdot Q(t_F,\rho) + \lambda^{V}(t_F,\rho)^{\mathrm{T}} \cdot V(t_F,\rho) + \lambda^{\Gamma}(t_F,\rho)^{\mathrm{T}} \cdot \Gamma(t_F,\rho) + \lambda^{Z}(t_F,\rho)^{\mathrm{T}} \cdot Z(t_F,\rho). \tag{3.18}$$

By comparing this equation with (3.10) one obtains the values of the adjoint variables at the final time t_F:

$$\lambda^{Q}(t_F,\rho) = \tilde{w}_q^{\mathrm{T}}\big|_{t_F}, \quad \lambda^{V}(t_F,\rho) = \tilde{w}_v^{\mathrm{T}}\big|_{t_F}, \quad \lambda^{\Gamma}(t_F,\rho) = \tilde{w}_\rho^{\mathrm{T}}\big|_{t_F}, \quad \lambda^{Z}(t_F,\rho) = \mathsf{I}_{n_c \times n_c}. \tag{3.19}$$

The equation (3.17) evaluated at $t = t_F$ leads to the direct sensitivity approach:

$$\begin{aligned} \frac{d\,\psi}{d\,\rho} &= \tilde{w}_q\big|_{t_F} \cdot Q(t_F,\rho) \,+\, \tilde{w}_v\big|_{t_F} \cdot V(t_F,\rho) \,+\, \tilde{w}_\rho\big|_{t_F} \cdot \mathsf{I}_{p\times p} \,+\, \mathsf{I}_{n_c\times n_c} \cdot Z(t_F,\rho) \\ &= \tilde{w}_q\big|_{t_F} \cdot Q(t_F,\rho) \,+\, \tilde{w}_v\big|_{t_F} \cdot V(t_F,\rho) \,+\, \tilde{w}_\rho\big|_{t_F} \,+\, Z(t_F,\rho). \end{aligned} \tag{3.20}$$

Evaluating (3.17) at $t = t_0$ leads to the adjoint sensitivity approach:

$$\begin{aligned} \frac{d\,\psi}{d\,\rho} &= \lambda^Q(t_0,\rho)^{\mathrm{T}} \cdot Q(t_0,\rho) + \lambda^V(t_0,\rho)^{\mathrm{T}} \cdot V(t_0,\rho) \;+\; \lambda^\Gamma(t_0,\rho)^{\mathrm{T}} \cdot \mathsf{I}_{p\times p} + \lambda^Z(t_0,\rho)^{\mathrm{T}} \cdot Z(t_0,\rho) \\ &= \lambda^Q(t_0,\rho)^{\mathrm{T}} \cdot \frac{dq_0(\rho)}{d\rho} \;+\; \lambda^V(t_0,\rho)^{\mathrm{T}} \cdot \frac{dv_0(\rho)}{d\rho} \;+\; \lambda^\Gamma(t_0,\rho)^{\mathrm{T}} \cdot \mathsf{I}_{p\times p} + \mathsf{I}_{n_c\times n_c} \cdot \mathsf{0}_{n_v\times n_c} \\ &= \lambda^Q(t_0,\rho)^{\mathrm{T}} \cdot \frac{dq_0(\rho)}{d\rho} \;+\; \lambda^V(t_0,\rho)^{\mathrm{T}} \cdot \frac{dv_0(\rho)}{d\rho} \;+\; \lambda^\Gamma(t_0,\rho)^{\mathrm{T}}. \end{aligned} \tag{3.21}$$

Note that the adjoint variables are initialized at $t = t_F$. However, their values at $t = t_0$ are the ones needed for computing the desired sensitivities.

Definition 3.1.4 (The canonical adjoint sensitivity for ODE systems)**.** The evolution of adjoint variables for ODE systems is governed by the following continuous adjoint model:

$$\begin{bmatrix} \dot\lambda^Q \\ \dot\lambda^V \\ \dot\lambda^\Gamma \\ \dot\lambda^Z \end{bmatrix} = - \begin{bmatrix} \mathsf{0}_{n\times n} & f_q^{\mathrm{eom}\,\mathrm{T}} & \mathsf{0}_{n\times p} & \tilde g_q^{\mathrm{T}} \\ \mathrm{I}_{n\times n} & f_v^{\mathrm{eom}\,\mathrm{T}} & \mathsf{0}_{n\times p} & \tilde g_v^{\mathrm{T}} \\ \mathsf{0}_{p\times n} & f_\rho^{\mathrm{eom}\,\mathrm{T}} & \mathsf{0}_{p\times p} & \tilde g_\rho^{\mathrm{T}} \\ \mathsf{0}_{n_c\times n} & \mathsf{0}_{n_c\times n} & \mathsf{0}_{n_c\times p} & \mathsf{0}_{n_c\times n_c} \end{bmatrix} \cdot \begin{bmatrix} \lambda^Q \\ \lambda^V \\ \lambda^\Gamma \\ \lambda^Z \end{bmatrix}, \quad t_F \ge t \ge t_0, \quad \lambda(t_F,\rho) := \begin{bmatrix} \tilde w_q^{\mathrm{T}}(t_F,\rho) \\ \tilde w_v^{\mathrm{T}}(t_F,\rho) \\ \tilde w_\rho^{\mathrm{T}}(t_F,\rho) \\ \mathrm{I}_{n_c\times n_c} \end{bmatrix} \in \mathbb{R}^{(2n+p+n_c)\times n_c}. \tag{3.22}$$

The adjoint sensitivities (3.22) are solved backward in time.

3.1.4 Hybrid ODE systems dynamics

In this study, we consider hybrid ODE systems characterized by piecewise-in-time smooth dynamics described by (3.1), and that exhibit discontinuous dynamic behavior (jump or non-smoothness) in the generalized velocity state vector at a finite number of time moments (no zeno phenomena [59]). Each such moment is corresponds to an event triggered by the event equation:

$$r\big(q|_{t_{\text{eve}}}\big) = 0, \tag{3.23}$$

where t_{eve} is the 'time of event' and $r : \mathbb{R}^n \to \mathbb{R}$ is a smooth 'event function'. Note that grazing phenomena are not considered the in this study. The following quantities are used to characterize an event:

- The value of a variable right before the event is denoted by $\boldsymbol{x}|^{-}_{t_{\text{eve}}} := \lim_{\varepsilon>0,\ \varepsilon\to 0} \boldsymbol{x}(t_{\text{eve}} - \varepsilon)$, and its value right after the event by $\boldsymbol{x}|^{+}_{t_{\text{eve}}} := \lim_{\varepsilon>0,\ \varepsilon\to 0} \boldsymbol{x}(t_{\text{eve}} + \varepsilon)$. The limits exist since the evolution of the system is smooth in time both before and after the event.

- The generalized position state variables remain the same after the event as before it, $q|^{+}_{t_{\text{eve}}} = q|^{-}_{t_{\text{eve}}} = q|_{t_{\text{eve}}}$. This is a consequence of the event changing the energy of the system by a finite amount.

- Also due to the finite energy change during the event, the quadrature variable is continuous in time, $\quad z|^{+}_{t_{\text{eve}}} = z|^{-}_{t_{\text{eve}}} = z|_{t_{\text{eve}}}$.

- An event that applies a finite energy impulse force to the system can abruptly change the generalized velocity state vector $\dot{q}$, from its value $v|^{-}_{t_{\text{eve}}}$ right before the event to a new value $v|^{+}_{t_{\text{eve}}}$ right after the event. The change in velocity is characterized by the 'jump function':

$$v|^{+}_{t_{\text{eve}}} = h\Big(t_{\text{eve}},\, q|_{t_{\text{eve}}},\, v|^{-}_{t_{\text{eve}}},\, \rho\Big) \quad \Leftrightarrow \quad \dot{q}|^{+}_{t_{\text{eve}}} = h\Big(t_{\text{eve}},\, q|_{t_{\text{eve}}},\, \dot{q}|^{-}_{t_{\text{eve}}},\, \rho\Big). \tag{3.24}$$

- An event where the system undergoes a sudden change of the equation of motions (3.1) at t_{eve} is characterized by the equations:

$$\begin{aligned} & \ddot{q}|^{-}_{t_{\text{eve}}} = f^{\text{eom}-}\big(t_{\text{eve}}, q|_{t_{\text{eve}}}, v|_{t_{\text{eve}}}, \rho\big) =: f^{\text{eom}-}|_{t_{\text{eve}}} \\ \xrightarrow{\text{event}} \quad & \ddot{q}|^{+}_{t_{\text{eve}}} = f^{\text{eom}+}\big(t_{\text{eve}}, q|_{t_{\text{eve}}}, v|_{t_{\text{eve}}}, \rho\big) =: f^{\text{eom}+}|_{t_{\text{eve}}}. \end{aligned} \tag{3.25}$$

Remark (Multiple events). In many cases, the change can be triggered by one of multiple events. Each individual event is described by the event function $r_\ell : \mathbb{R}^n \to \mathbb{R}$, $\ell = 1, \ldots, e$. The detection of the next event (3.23), which can be one of the possible e options, is described by $\Pi_{i=1}^{e} r_i\big(q|_{t_{\text{eve}}}\big) = 0$, and if event ℓ takes place, then $r_\ell = 0$ and the corresponding jump in velocity (3.24) is $v|^{+}_{t_{\text{eve}}} = h_\ell\Big(q|_{t_{\text{eve}}},\, v|^{-}_{t_{\text{eve}}}\Big)$, or the corresponding change in the equations of motion (3.25) is $\ddot{q}|^{+}_{t_{\text{eve}}} =: f^{\text{eom}+}_{\ell}|_{t_{\text{eve}}}$.

3.1.5 Direct sensitivity analysis for hybrid ODE systems

Let $Q|^{+}_{t_{\text{eve}}}$ and $Q|^{-}_{t_{\text{eve}}} \in \mathbb{R}^{n \times p}$ be the sensitivities of the generalized position state matrix after and before the event, respectively. Let $V|^{+}_{t_{\text{eve}}}, V|^{-}_{t_{\text{eve}}} \in \mathbb{R}^{n \times p}$ be the sensitivities of the generalized velocity state matrix after and before the event, respectively. Let $Z|^{+}_{t_{\text{eve}}}$ and $Z|^{-}_{t_{\text{eve}}}$, with $Z \in \mathbb{R}^{p}$, be the sensitivities of the quadrature variable $z(t)$ after and before the event, respectively. It is shown in [64] that, at the time of the event, we have:

- The sensitivity of the time of event with respect to the system parameters is:

$$\frac{dt_{\text{eve}}}{d\rho} = -\frac{\dfrac{dr}{dq}\left(q|_{t_{\text{eve}}}\right) \cdot Q|^{-}_{t_{\text{eve}}}}{\dfrac{dr}{dq}\left(q|_{t_{\text{eve}}}\right) \cdot v|^{-}_{t_{\text{eve}}}} \in \mathbb{R}^{1\times p}. \tag{3.26a}$$

  where $dr/dq \in \mathbb{R}^{1\times n}$ is the Jacobian of the event function.

- The jump equation of the sensitivities of the generalized position state vector is:

$$Q|^{+}_{t_{\text{eve}}} = Q|^{-}_{t_{\text{eve}}} - \left(v|^{+}_{t_{\text{eve}}} - v|^{-}_{t_{\text{eve}}}\right) \cdot \frac{dt_{\text{eve}}}{d\rho}. \tag{3.26b}$$

- The jump equation of the sensitivities of the generalized velocity state vector is:

$$\begin{aligned} V|^{+}_{t_{\text{eve}}} =& h_q|^{-}_{t_{\text{eve}}} \cdot Q|^{-}_{t_{\text{eve}}} + h_v|^{-}_{t_{\text{eve}}} \cdot V|^{-}_{t_{\text{eve}}} \\ &+ \left(h_q|^{-}_{t_{\text{eve}}} \cdot v|^{-}_{t_{\text{eve}}} - \ddot{q}|^{+}_{t_{\text{eve}}} + h_v|^{-}_{t_{\text{eve}}} \cdot \ddot{q}|^{-}_{t_{\text{eve}}} + h_t|^{-}_{t_{\text{eve}}}\right) \cdot \frac{dt_{\text{eve}}}{d\rho} + h_\rho|^{-}_{t_{\text{eve}}}, \end{aligned} \tag{3.26c}$$

  where the Jacobians of the jump function are:

$$\begin{aligned} h_t|^{-}_{t_{\text{eve}}} &:= \tfrac{\partial h}{\partial t}\left(t_{\text{eve}}, q|_{t_{\text{eve}}}, v|^{-}_{t_{\text{eve}}}, \rho\right) \in \mathbb{R}^{f\times 1}, & h_q|^{-}_{t_{\text{eve}}} &:= \frac{\partial h}{\partial q}\left(t_{\text{eve}}, q|_{t_{\text{eve}}}, v|^{-}_{t_{\text{eve}}}, \rho\right) \in \mathbb{R}^{f\times n}, \\ h_v|^{-}_{t_{\text{eve}}} &:= \tfrac{\partial h}{\partial v}\left(t_{\text{eve}}, q|_{t_{\text{eve}}}, v|^{-}_{t_{\text{eve}}}, \rho\right) \in \mathbb{R}^{f\times f}, & h_\rho|^{-}_{t_{\text{eve}}} &:= \frac{\partial h}{\partial \rho}\left(t_{\text{eve}}, q|_{t_{\text{eve}}}, v|^{-}_{t_{\text{eve}}}, \rho\right) \in \mathbb{R}^{f\times p}. \end{aligned} \tag{3.26d}$$

- The sensitivity of the cost function changes during the event is :

$$Z|_{t_{\mathrm{eve}}}^{+} = Z|_{t_{\mathrm{eve}}}^{-} - \Big(g|_{t_{\mathrm{eve}}}^{+} - g|_{t_{\mathrm{eve}}}^{-}\Big) \cdot \frac{dt_{\mathrm{eve}}}{d\rho}. \tag{3.26e}$$

  where

$$g|_{t_{\mathrm{eve}}}^{+} := \tilde{g}\big(t_{\mathrm{eve}}, q|_{t_{\mathrm{eve}}}, v|_{t_{\mathrm{eve}}}^{+}, \rho\big), \quad g|_{t_{\mathrm{eve}}}^{-} := \tilde{g}\big(t_{\mathrm{eve}}, q|_{t_{\mathrm{eve}}}, v|_{t_{\mathrm{eve}}}^{-}, \rho\big), \tag{3.26f}$$

  is the running cost function evaluated right after and right before the event, respectively.

Definition 3.1.5 (The generalized jump sensitivity matrix)**.** The direct sensitivity jump equations (3.26) can be written compactly in matrix form as $X|_{t_{\mathrm{eve}}}^{+} = S \cdot X|_{t_{\mathrm{eve}}}^{-}$, where S is the generalized sensitivity jump matrix:

$$\begin{bmatrix} Q|_{t_{\mathrm{eve}}}^{+} \\ V|_{t_{\mathrm{eve}}}^{+} \\ \Gamma|_{t_{\mathrm{eve}}}^{+} \\ Z|_{t_{\mathrm{eve}}}^{+} \end{bmatrix} = \underbrace{\begin{bmatrix} \big(Q|_{t_{\mathrm{eve}}}^{+}\big)_{Q|_{t_{\mathrm{eve}}}^{-}} & \mathsf{0}_{n\times n} & \mathsf{0}_{n\times p} & \mathsf{0}_{n\times n_c} \\ \big(V|_{t_{\mathrm{eve}}}^{+}\big)_{Q|_{t_{\mathrm{eve}}}^{-}} & h_v|_{t_{\mathrm{eve}}}^{-} & h_\rho|_{t_{\mathrm{eve}}}^{-} & \mathsf{0}_{n\times n_c} \\ \mathsf{0}_{p\times n} & \mathsf{0}_{p\times n} & \mathsf{I}_{p\times p} & \mathsf{0}_{p\times n_c} \\ \big(Z|_{t_{\mathrm{eve}}}^{+}\big)_{Q|_{t_{\mathrm{eve}}}^{-}} & \mathsf{0}_{n_c\times n} & \mathsf{0}_{n_c\times p} & \mathsf{I}_{n_c\times n_c} \end{bmatrix}}_{\mathsf{S}_{\mathrm{eve}}} \cdot \begin{bmatrix} Q|_{t_{\mathrm{eve}}}^{-} \\ V|_{t_{\mathrm{eve}}}^{-} \\ \Gamma|_{t_{\mathrm{eve}}}^{-} \\ Z|_{t_{\mathrm{eve}}}^{-} \end{bmatrix}. \tag{3.27a}$$

The Jacobians $\big(Q|_{t_{\mathrm{eve}}}^{+}\big)_{Q|_{t_{\mathrm{eve}}}^{-}}$ and $\big(V|_{t_{\mathrm{eve}}}^{+}\big)_{Q|_{t_{\mathrm{eve}}}^{-}}$ are:

$$\big(Q|_{t_{\mathrm{eve}}}^{+}\big)_{Q|_{t_{\mathrm{eve}}}^{-}} = \mathrm{I} - \left(\mathrm{v}|_{\mathrm{t_{eve}}}^{+} - \mathrm{v}|_{\mathrm{t_{eve}}}^{-}\right) \cdot \left(\frac{\mathrm{dt_{eve}}}{\mathrm{d}\rho}\right)_{\mathrm{Q}|_{\mathrm{t_{eve}}}^{-}} \in \mathbb{R}^{\mathrm{n}\times\mathrm{n}}, \tag{3.27b}$$

$$\begin{aligned}\left(V|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}} =& h_q|_{t_{\text{eve}}}^{-} + \\ & \left(h_q|_{t_{\text{eve}}}^{-} \cdot v|_{t_{\text{eve}}}^{-} - \ddot{q}|_{t_{\text{eve}}}^{+} + h_v|_{t_{\text{eve}}}^{-} \cdot \ddot{q}|_{t_{\text{eve}}}^{-} + h_t|_{t_{\text{eve}}}^{-}\right) \cdot \left(\frac{dt_{\text{eve}}}{d\rho}\right)_{Q|_{t_{\text{eve}}}^{-}} \in \mathbb{R}^{n \times n},\end{aligned} \tag{3.27c}$$

with,

$$\left(\frac{dt_{\text{eve}}}{d\rho}\right)_{Q|_{t_{\text{eve}}}^{-}} = - \frac{\dfrac{dr}{dq}\left(q|_{t_{\text{eve}}}\right)}{\dfrac{dr}{dq}\left(q|_{t_{\text{eve}}}\right) \cdot v|_{t_{\text{eve}}}^{-}} \in \mathbb{R}^{1 \times n}. \tag{3.27d}$$

The Jacobian $\left(Z|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}$ is:

$$\left(Z|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}} = - \left(g|_{t_{\text{eve}}}^{+} - g|_{t_{\text{eve}}}^{-}\right) \cdot \left(\frac{dt_{\text{eve}}}{d\rho}\right)_{Q|_{t_{\text{eve}}}^{-}} \in \mathbb{R}^{n_c \times n}. \tag{3.27e}$$

3.1.6 Adjoint sensitivity analysis for hybrid ODE unconstrained dynamical systems

Theorem 9 (Adjoint sensitivity jump matrix)**.** *Let* $\lambda^Q|_{t_{\text{eve}}}^{-} \in \mathbb{R}^{n \times n_c}$, $\lambda^V|_{t_{\text{eve}}}^{-} \in \mathbb{R}^{n \times n_c}$, $\lambda^\Gamma|_{t_{\text{eve}}}^{-} \in \mathbb{R}^{p \times n_c}$ *and* $\lambda^Z|_{t_{\text{eve}}}^{-} \in \mathbb{R}^{n_c \times n_c}$ *be the adjoint sensitivities before the time of event respectively, and* $\lambda|_{t_{\text{eve}}}^{-} = \begin{bmatrix}\lambda^Q|_{t_{\text{eve}}}^{-\,\mathrm{T}} & \lambda^V|_{t_{\text{eve}}}^{-\,\mathrm{T}} & \lambda^\Gamma|_{t_{\text{eve}}}^{-\,\mathrm{T}} & \lambda^Z|_{t_{\text{eve}}}^{-\,\mathrm{T}}\end{bmatrix}^{\mathrm{T}}$*. Let* $\lambda^Q|_{t_{\text{eve}}}^{+} \in \mathbb{R}^{n \times n_c}$, $\lambda^V|_{t_{\text{eve}}}^{+} \in \mathbb{R}^{n \times n_c}$, $\lambda^\Gamma|_{t_{\text{eve}}}^{+} \in \mathbb{R}^{p \times n_c}$ *and* $\lambda^Z|_{t_{\text{eve}}}^{+} \in \mathbb{R}^{n_c \times n_c}$ *be the adjoint sensitivities after the time of event respectively, and* $\lambda|_{t_{\text{eve}}}^{+} = \begin{bmatrix}\lambda^Q|_{t_{\text{eve}}}^{+\,\mathrm{T}} & \lambda^V|_{t_{\text{eve}}}^{+\,\mathrm{T}} & \lambda^\Gamma|_{t_{\text{eve}}}^{+\,\mathrm{T}} & \lambda^Z|_{t_{\text{eve}}}^{+\,\mathrm{T}}\end{bmatrix}^{\mathrm{T}}$.

The adjoint sensitivity jump equations at the time of an event are:

$$\lambda|_{t_{\text{eve}}}^{-} = \mathsf{S}_{\text{eve}}^{T} \cdot \lambda|_{t_{\text{eve}}}^{+} \in \mathbb{R}^{(2\times n+p+n_c)\times n_c} \tag{3.28}$$

where $\mathsf{S}_{\text{eve}}^{T}$ *is the transpose of the generalized sensitivity jump matrix* (3.27a).

Proof. We start the proof from the following statement provided in [44] that mentions that the dot product of the sensitivity state matrix with the adjoint sensitive state matrix is constant at any time, ${\lambda|_{t_{\text{eve}}}^{+}}^{\mathrm{T}} \cdot {X|_{t_{\text{eve}}}^{+}}^{\mathrm{T}} = {\lambda|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} \cdot {X|_{t_{\text{eve}}}^{-}}^{\mathrm{T}}$. Using (3.27a), the previous relationship is equivalent to ${\lambda|_{t_{\text{eve}}}^{+}}^{\mathrm{T}} \cdot \mathsf{S}_{\text{eve}} \cdot {X|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} = {\lambda|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} \cdot {X|_{t_{\text{eve}}}^{-}}^{\mathrm{T}}$. Since this holds for any matrix $X|_{t_{\text{eve}}}^{-}$ it follows that ${\lambda|_{t_{\text{eve}}}^{+}}^{\mathrm{T}} \cdot \mathsf{S}_{\text{eve}} = {\lambda|_{t_{\text{eve}}}^{-}}^{\mathrm{T}}$, which is equivalent to (3.28). □

Remark. From (3.27a) and (3.28) the adjoint sensitivity jump equations for ODE systems without constraints are:

$$\lambda^{Q}|_{t_{\text{eve}}}^{-} = \left(Q|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} \cdot \lambda^{Q}|_{t_{\text{eve}}}^{+} + \left(V|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} \cdot \lambda^{V}|_{t_{\text{eve}}}^{+} + \left(Z|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} \cdot \lambda^{Z}|_{t_{\text{eve}}}^{+} \tag{3.29a}$$

$$\lambda^{V}|_{t_{\text{eve}}}^{-} = (h_v|_{t_{\text{eve}}}^{-})^{\mathrm{T}} \cdot \lambda^{V}|_{t_{\text{eve}}}^{+} \tag{3.29b}$$

$$\lambda^{\Gamma}|_{t_{\text{eve}}}^{-} = (h_\rho|_{t_{\text{eve}}}^{-})^{\mathrm{T}} \cdot \lambda^{V}|_{t_{\text{eve}}}^{+} + \lambda^{\Gamma}|_{t_{\text{eve}}}^{+} \tag{3.29c}$$

$$\lambda^{Z}|_{t_{\text{eve}}}^{-} = \lambda^{Z}|_{t_{\text{eve}}}^{+} \tag{3.29d}$$

3.2 Sensitivity analysis for constrained multibody dynamical systems and extended cost functions

3.2.1 Representation of constrained multibody systems

We consider constrained multibody systems that satisfy the following kinematic constraints:

$$
\begin{aligned}
\mathsf{0} &= \Phi, && (3.30a)\\
\mathsf{0} &= \dot{\Phi} = \Phi_q\,\dot{q} + \Phi_t \quad \Rightarrow \quad \Phi_q v = -\Phi_t, && (3.30b)\\
\mathsf{0} &= \ddot{\Phi} = \Phi_q\,\ddot{q} + \Phi_{q,q}\,(\dot{q},\dot{q}) + \Phi_{t,q}\,\dot{q} + \Phi_{t,t} && (3.30c)\\
&\Rightarrow \quad \Phi_q\,\dot{v} = -(\Phi_q\,v)\,v - \Phi_{t,q}\,v - \Phi_{t,t} := \mathsf{C}. && (3.30d)
\end{aligned}
$$

Here (3.30a) is a holonomic position constraint equation $\Phi(t,q,\rho) = \mathsf{0}$, where $\Phi : \mathbb{R}^{1+n+p} \to \mathbb{R}^m$ is a smooth 'position constraint' function. The velocity (3.30b) and the acceleration (3.30c) kinematic constraints are found by differentiating the position constraint with respect to time.

Remark. Formalisms for constrained multibody systems may involve Lagrangian coefficients $\mu : \mathbb{R}^{1+2n+p} \to \mathbb{R}^m$ that provide the necessary forces to satisfy the kinematic constraints [64]. Our notation encompasses the case where the cost function penalizes the accelerations $\dot{v}$ and the joint forces via the Lagrangian coefficients μ:

$$\tilde{g}\big(t,\, q,\, v,\, \rho\big) = g\big(t,\, q,\, v,\, \dot{v}(t,\, q,\, v,\, \rho),\, \rho,\, \mu(t,\, q,\, v,\, \rho)\big). \tag{3.31}$$

It is shown in 3.3 that the terminal cost function $\tilde{w}$ cannot directly depend on the acceleration $\dot{v}$ or on the Lagrange coefficients μ, and therefore the derivatives are $\tilde{w}_{\dot{v}} = 0$ and $\tilde{w}_{\mu} = 0$. In a different notation, such result is also shown in [1]. Using equation (3.10) we see that the final condition for the adjoint of the algebraic variables μ is zero, $\lambda^{\Lambda}_{t_F} = \tilde{w}_{\mu}\big|_{t_F} = 0$.

3.2.2 Direct and adjoint sensitivity analysis for smooth systems in the penalty ODE formulation

Define the extended mass matrix $\overline{\mathsf{M}} : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^{n \times n}$ and the extended right hand side function $\overline{\mathsf{F}} : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^n$ as:

$$\overline{\mathsf{M}}\,(t, q, v, \rho) := \mathsf{M}\,(t, q, v, \rho) + \Phi_q^{\mathrm{T}}\,(t, q, v, \rho) \cdot \alpha \cdot \Phi_q\,(t, q, v, \rho)\,, \tag{3.32}$$

$$\overline{\mathsf{F}}\,(t, q, v, \rho) := \mathsf{F}\,(t, q, v, \rho) - \Phi_q^{\mathrm{T}} \cdot \alpha \cdot \Big(\dot{\Phi}_q\, v + \dot{\Phi}_t + 2\,\xi\,\omega\,\dot{\Phi} + \omega^2\Phi\Big)\,, \tag{3.33}$$

where $\alpha \in \mathbb{R}^{m \times m}$ is the penalty factor of the ODE penalty formulation, $\xi \in \mathbb{R}$ and $\omega \in \mathbb{R}$ are the natural frequency and damping ratio coefficients of the formulation, respectively. The functions Φ, $\dot{\Phi}$, $\ddot{\Phi} : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^p \to \mathbb{R}^m$ are the position, velocity and acceleration kinematic constraints, respectively. The penalty formulation of a constrained rigid multibody system is written as a first order ODE:

$$\begin{cases} \dot{q} &= v, \\ \dot{v} &= f^{\textrm{eom}}(t,\, q,\, v,\, \rho) = \overline{\mathsf{M}}^{-1}(t,\, q,\, v,\, \rho) \cdot \overline{\mathsf{F}}(t,\, q,\, v,\, \rho). \end{cases} \tag{3.34}$$

The Lagrange multipliers associated to the constraint forces are estimated as $\mu^* = \alpha\, \left(\ddot{\Phi} + 2\,\xi\,\omega\,\dot{\Phi} + \omega^2\,\Phi \right)$. The sensitivities of the state variables of the system with respect to parameters evolve according to the tangent linear model derived in [58, 29, 1, 27, 2]. Since the penalty formulation (3.34) evolves as an ODE, we can compute the direct sensitivities using (3.11) with $f^{\textrm{eom}}_q = \overline{\mathsf{F}}_q - \overline{\mathsf{M}}_q\,\dot{v}$, $f^{\textrm{eom}}_v = \overline{\mathsf{F}}_v$, $f^{\textrm{eom}}_\rho = \overline{\mathsf{F}}_\rho - \overline{\mathsf{M}}_\rho\,\dot{v}$, as shown in Appendix B. The derivatives $\overline{\mathsf{M}}_\rho$, $\overline{\mathsf{M}}_q$, $\overline{\mathsf{F}}_q$, $\overline{\mathsf{F}}_v$, and $\overline{\mathsf{F}}_\rho$ are given in [64]. Similarly, one can compute the adjoint sensitivities of the penalty formulation (3.34) using (3.22).

3.2.3 Direct and adjoint sensitivity analysis for smooth systems in the index-1 differential-algebraic formulation

Definition 3.2.1 (Constrained multibody dynamics: the index-1 DAE formulation)**.** The index-1 formulation of the equations of motion is obtained by replacing the position constraint (3.30a) with the acceleration constraint (3.30c):

$$\begin{bmatrix} \mathsf{I} & \mathsf{0} & \mathsf{0} \\ \mathsf{0} & \mathsf{M}\left(t,q,\rho\right) & \Phi_q^{\mathrm{T}}\left(t,q,\rho\right) \\ \mathsf{0} & \Phi_q\left(t,q,\rho\right) & \mathsf{0} \end{bmatrix} \cdot \begin{bmatrix} \dot{q} \\ \dot{v} \\ \mu \end{bmatrix} = \begin{bmatrix} v \\ \mathsf{F}\left(t,q,v,\rho\right) \\ \mathsf{C}\left(t,q,v,\rho\right) \end{bmatrix}, \quad t_0 \le t \le t_F, \tag{3.35}$$

with $q(t_0) = q_0(\rho), \quad v(t_0) = v_0(\rho)$. The algebraic equation has the form $f^{\text{DAE-}\mu} - \mu = 0$.

Definition 3.2.2 (Tangent linear index-1 DAE)**.** Sensitivities of solutions (3.8) and multipliers:

$$\Lambda_i(t,\rho) := \frac{d\,\mu(t,\rho)}{d\,\rho_i} \in \mathbb{R}^m, \quad i = 1, \ldots, p; \tag{3.36}$$

of the system (3.35) with respect to parameters evolve according to the tangent linear model derived in [58, 29, 1, 27, 2]:

$$\begin{bmatrix} \dot{Q} \\ \dot{V} \\ \dot{\Gamma} \\ \Lambda \\ \dot{Z} \end{bmatrix} = \begin{bmatrix} V \\ f_q^{\text{DAE-}\dot{v}} Q + f_v^{\text{DAE-}\dot{v}} V + f_\rho^{\text{DAE-}\dot{v}} \\ \mathsf{0}_{p\times p} \\ f_q^{\text{DAE-}\mu} Q + f_v^{\text{DAE-}\mu} V + f_\rho^{\text{DAE-}\mu} \\ \left(g_q + g_{\dot{v}}\, f_q^{\text{DAE-}\dot{v}} + g_\mu\, f_q^{\text{DAE-}\mu}\right) \cdot Q + \left(g_v + g_{\dot{v}}\, f_v^{\text{DAE-}\dot{v}} + g_\mu\, f_v^{\text{DAE-}\mu}\right) \cdot V + \left(g_\rho + g_{\dot{v}}\, f_\rho^{\text{DAE-}\dot{v}} + g_\mu\, f_\rho^{\text{DAE-}\mu}\right) \end{bmatrix} \tag{3.37}$$

It is shown in Appendix B, that equation (3.37) can be written in matrix form as follows:

$$\begin{bmatrix} \dot{Q} \\ \dot{V} \\ \dot{\Gamma} \\ \Lambda \\ \dot{Z} \end{bmatrix} = \begin{bmatrix} \mathsf{0}_{n\times n} & \mathsf{I}_{n\times n} & \mathsf{0}_{n\times p} & \mathsf{0}_{n\times m} & \mathsf{0}_{n\times n_c} \\ f_q^{\text{DAE-}\dot{v}} & f_v^{\text{DAE-}\dot{v}} & f_\rho^{\text{DAE-}\dot{v}} & \mathsf{0}_{n\times m} & \mathsf{0}_{n\times n_c} \\ \mathsf{0}_{p\times n} & \mathsf{0}_{p\times n} & \mathsf{0}_{p\times p} & \mathsf{0}_{p\times m} & \mathsf{0}_{p\times n_c} \\ f_q^{\text{DAE-}\mu} & f_v^{\text{DAE-}\mu} & f_\rho^{\text{DAE-}\mu} & \mathsf{0}_{m\times m} & \mathsf{0}_{m\times n_c} \\ \tilde{g}_q & \tilde{g}_v & \tilde{g}_\rho & \mathsf{0}_{n_c\times m} & \mathsf{0}_{n_c\times n_c} \end{bmatrix} \cdot \begin{bmatrix} Q \\ V \\ \Gamma \\ \Lambda \\ Z \end{bmatrix}, \tag{3.38}$$

with initial conditions given by Eq. (3.9). Using Appendix B, the derivatives of the DAE function are:

$$f_q^{\text{DAE}} = \begin{bmatrix} \mathsf{M} & \Phi_q^{\mathrm{T}} \\ \Phi_q & \mathsf{0} \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{F}_q - \mathsf{M}_q\,\dot{v} - \Phi_{q,\,q}^{\mathrm{T}}\,\mu \\ \mathsf{C}_q - \Phi_{q,\,q}\dot{v} \end{bmatrix}, \; f_v^{\text{DAE}} = \begin{bmatrix} \mathsf{M} & \Phi_q^{\mathrm{T}} \\ \Phi_q & \mathsf{0} \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{F}_v \\ \mathsf{C}_v \end{bmatrix} \tag{3.39}$$

$$f_\rho^{\text{DAE}} = \begin{bmatrix} \mathsf{M} & \Phi_q^{\mathrm{T}} \\ \Phi_q & \mathsf{0} \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{F}_\rho - \mathsf{M}_\rho\,\dot{v} - \Phi_{q,\,\rho}^{T}\,\mu \\ \mathsf{C}_\rho - \Phi_{q,\,\rho}\,\dot{v} \end{bmatrix}.$$

Definition 3.2.3 (Continuous adjoint index-1 DAE systems)**.** The continuous adjoint differential equation corresponding to the index-1 DAE tangent linear model (3.38) is:

$$\begin{bmatrix} \dot{\lambda}^{Q} \\ \dot{\lambda}^{V} \\ \dot{\lambda}^{\Gamma} \\ \lambda^{\Lambda} \\ \dot{\lambda}^{Z} \end{bmatrix} = - \begin{bmatrix} \mathsf{0}_{n\times n} & f_q^{\text{DAE-}\dot{v}\,\mathrm{T}} & \mathsf{0}_{n\times p} & f_q^{\text{DAE-}\mu\,\mathrm{T}} & \tilde{g}_q^{\mathrm{T}} \\ \mathsf{I}_{n\times n} & f_v^{\text{DAE-}\dot{v}\,\mathrm{T}} & \mathsf{0}_{n\times p} & f_v^{\text{DAE-}\mu\,\mathrm{T}} & \tilde{g}_v^{\mathrm{T}} \\ \mathsf{0}_{p\times n} & f_\rho^{\text{DAE-}\dot{v}\,\mathrm{T}} & \mathsf{0}_{p\times p} & f_\rho^{\text{DAE-}\mu\,\mathrm{T}} & \tilde{g}_\rho^{\mathrm{T}} \\ \mathsf{0}_{m\times n} & \mathsf{0}_{m\times n} & \mathsf{0}_{m\times p} & \mathsf{0}_{m\times m} & \mathsf{0}_{m\times n_c} \\ \mathsf{0}_{n_c\times n} & \mathsf{0}_{n_c\times n} & \mathsf{0}_{n_c\times p} & \mathsf{0}_{n_c\times m} & \mathsf{0}_{n_c\times n_c} \end{bmatrix} \cdot \begin{bmatrix} \lambda^{Q} \\ \lambda^{V} \\ \lambda^{\Gamma} \\ \lambda^{\Lambda} \\ \lambda^{Z} \end{bmatrix}, \quad t_F \geq t \geq t_0. \tag{3.40}$$

with, $\lambda(t_F, \rho) := \begin{bmatrix} \tilde{w}_q(t_F, \rho) & \tilde{w}_v(t_F, \rho) & \tilde{w}_\rho(t_F, \rho) & 0_{n_c\times m} & \mathrm{I}_{n_c\times n_c} \end{bmatrix}^{\mathrm{T}} \in \mathbb{R}^{(2n+p+m+n_c)\times n_c}$.

Noting from remark 3.2.1 that the algebraic equation in (3.40) reads:

$$\lambda^{\Lambda}(t) = 0, \quad t_F \geq t \geq t_0,$$

the index-1 adjoint DAE (3.40) can be reduced to the following adjoint ODE:

$$\begin{bmatrix} \dot{\lambda}^{Q} \\ \dot{\lambda}^{V} \\ \dot{\lambda}^{\Gamma} \\ \dot{\lambda}^{Z} \end{bmatrix} = - \begin{bmatrix} \mathsf{0}_{n\times n} & f_q^{\text{DAE-}\dot{v}\,\mathrm{T}} & \mathsf{0}_{n\times p} & \tilde{g}_q^{\mathrm{T}} \\ \mathsf{I}_{n\times n} & f_v^{\text{DAE-}\dot{v}\,\mathrm{T}} & \mathsf{0}_{n\times p} & \tilde{g}_v^{\mathrm{T}} \\ \mathsf{0}_{p\times n} & f_\rho^{\text{DAE-}\dot{v}\,\mathrm{T}} & \mathsf{0}_{p\times p} & \tilde{g}_\rho^{\mathrm{T}} \\ \mathsf{0}_{n_c\times n} & \mathsf{0}_{n_c\times n} & \mathsf{0}_{n_c\times p} & \mathsf{0}_{n_c\times n_c} \end{bmatrix} \cdot \begin{bmatrix} \lambda^{Q} \\ \lambda^{V} \\ \lambda^{\Gamma} \\ \lambda^{Z} \end{bmatrix}, \quad t_F \geq t \geq t_0, \tag{3.41}$$

with $\lambda(t_F, \rho) := \begin{bmatrix} \tilde{w}_q(t_F, \rho) & \tilde{w}_v(t_F, \rho) & \tilde{w}_\rho(t_F, \rho) & \mathrm{I}_{n_c\times n_c} \end{bmatrix}^{\mathrm{T}} \in \mathbb{R}^{(2n+p+m+n_c)\times n_c}$.

3.2.4 Direct sensitivity analysis for hybrid constrained dynamical systems

We now discuss constrained dynamical systems when the dynamics is piecewise smooth in time. Performing a sensitivity analysis for a constrained rigid hybrid multibody dynamic system requires finding the jump conditions at the time of event. These jump equations are explained in our previous work [64]. We summarize below the jump equations at the time of event:

- The generalized position state variables remain the same , i.e., $q|_{t_{\text{eve}}}^{+} = q|_{t_{\text{eve}}}^{-} = q|_{t_{\text{eve}}}$ and need to satisfy both constraint functions $\Phi^{-}|_{t_{\text{eve}}}^{-} := \Phi^{-}\left(t_{\text{eve}}, q|_{t_{\text{eve}}}, \rho\right) = 0$, and $\Phi^{+}|_{t_{\text{eve}}}^{+} := \Phi^{+}\left(t_{\text{eve}}, q|_{t_{\text{eve}}}, \rho\right) = 0$.

- The velocity state variables jump from their values right before the event to right after the event according to the jump equation:

  $$v_{\text{dof+}}|_{t_{\text{eve}}}^{+} = h\Big(t_{\text{eve}}, q|_{t_{\text{eve}}}, v_{\text{dof-}}|_{t_{\text{eve}}}^{-}, \rho\Big), \qquad h : \mathbb{R}^{1+n+f^{-}+p} \rightarrow \mathbb{R}^{f^{+}}. \tag{3.42}$$

  The jump function (3.42) is assumed to be smooth and defined in terms of the velocity degrees of freedom (the independent components).

- The jumps in velocity cannot be arbitrary for the dependent components. They are dependent of the degree of freedom and are obtained from solving the velocity constraints leading to:

$$\begin{aligned} v_{\text{dep}+}\big|^{+}_{t_{\text{eve}}} &= -\left(\Phi^{+}_{q_{\text{dep}+}}\big|^{+}_{t_{\text{eve}}}\right)^{-1} \cdot \left(\Phi^{+}_{q_{\text{dof}+}}\big|^{+}_{t_{\text{eve}}} v_{\text{dof}+}\big|^{+}_{t_{\text{eve}}} + \Phi^{+}_{t}\big|^{+}_{t_{\text{eve}}}\right) \\ &= \mathsf{R}^{+}\big|^{+}_{t_{\text{eve}}} v_{\text{dof}+}\big|^{+}_{t_{\text{eve}}} - \left(\Phi^{+}_{q_{\text{dep}+}}\big|^{+}_{t_{\text{eve}}}\right)^{-1} \cdot \Phi^{+}_{t}\big|^{+}_{t_{\text{eve}}}. \end{aligned} \tag{3.43}$$

Where $\mathsf{R}^{\pm}$ corresponds to the null space of the constraints if the constraints are scleronomic (non explicitly time dependent).

There are two types of velocity jumps that our formalism covers (3.42)–(3.43):

- The case where the event consists of an elastic contact/collision/impact on the DOF components of the velocity state. The impulsive (external) contact forces act to change the DOF components without changing the set of constraint equations, $\Phi^{+} \equiv \Phi^{-}$.
- The case where the event consists solely of an inelastic collisions and a change of constraints $\Phi^{+} \neq \Phi^{-}$, without any external force modifying the independent velocities. The impulsive (internal) constraints forces at the time of event are solved by using a popular approach in robotics [31]:

$$\begin{bmatrix} \mathsf{M}\big|_{t_{\text{eve}}} & (\Phi^{+}_{q})^{\mathrm{T}}\big|_{t_{\text{eve}}} \\ \Phi^{+}_{q}\big|_{t_{\text{eve}}} & \mathsf{0} \end{bmatrix} \cdot \begin{bmatrix} v\big|^{+}_{t_{\text{eve}}} \\ \delta\mu \end{bmatrix} = \begin{bmatrix} \mathsf{M}\big|_{t_{\text{eve}}} \cdot v\big|^{-}_{t_{\text{eve}}} \\ -\Phi^{+}_{t}\big|_{t_{\text{eve}}} \end{bmatrix}, \tag{3.44a}$$

or, equivalently,

$$\begin{bmatrix} v|^{+}_{t_{\text{eve}}} \\ \delta\mu \end{bmatrix} = \begin{bmatrix} \mathsf{M}|_{t_{\text{eve}}} & (\Phi^{+}_{q})^{\mathrm{T}}|_{t_{\text{eve}}} \\ \Phi^{+}_{q}|_{t_{\text{eve}}} & \mathsf{0} \end{bmatrix}^{-1} \cdot \begin{bmatrix} \mathsf{M}|_{t_{\text{eve}}} \cdot v|^{-}_{t_{\text{eve}}} \\ -\Phi^{+}_{t}|_{t_{\text{eve}}} \end{bmatrix} = \begin{bmatrix} f^{\text{DAE-imp-}v}\big(t_{\text{eve}},\, q|_{t_{\text{eve}}},\, v|^{-}_{t_{\text{eve}}},\, \rho\big) \\ f^{\text{DAE-imp-}\mu}\big(t_{\text{eve}},\, q|_{t_{\text{eve}}},\, v|^{-}_{t_{\text{eve}}},\, \rho\big) \end{bmatrix}. \tag{3.44b}$$

The second equation (3.44b) imposes the velocity constraint on both independent and dependent coordinates, which is covered by our formalism as:

$$v_{\text{dof}+}|^{+}_{t_{\text{eve}}} = \mathsf{P}_{\text{dof}+}\, f^{\text{DAE-imp-}v}\big(t_{\text{eve}},\, q|_{t_{\text{eve}}},\, v|^{-}_{t_{\text{eve}}},\, \rho\big) =: h\left(t_{\text{eve}},\, q|_{t_{\text{eve}}},\, v_{\text{dof}-}|^{-}_{t_{\text{eve}}},\, \rho\right), \tag{3.45}$$

where $\mathsf{P} = \begin{bmatrix} \mathsf{P}^{\mathrm{T}}_{\text{dep}} & \mathsf{P}^{\mathrm{T}}_{\text{dof}} \end{bmatrix}^{\mathrm{T}}$ is a permutation matrix that partitions the state variables into dependent and independent variables.

Finally, the jump conditions at the time of event in the sensitivity state matrix are:

- The independent components of the sensitivity of the generalized positions right after the event:

$$Q_{\text{dof}+}|^{+}_{t_{\text{eve}}} = Q_{\text{dof}+}|^{-}_{t_{\text{eve}}} - \left(v_{\text{dof}+}|^{+}_{t_{\text{eve}}} - v_{\text{dof}+}|^{-}_{t_{\text{eve}}}\right) \cdot \frac{dt_{\text{eve}}}{d\rho}. \tag{3.46a}$$

which are equivalent to:

$$\mathsf{P}^{+}_{\text{dof}+} \cdot \left(Q|^{+}_{t_{\text{eve}}} - Q|^{-}_{t_{\text{eve}}}\right) = -\mathsf{P}^{+}_{\text{dof}+} \cdot \left(v|^{+}_{t_{\text{eve}}} - v|^{-}_{t_{\text{eve}}}\right) \cdot \frac{dt_{\text{eve}}}{d\rho}. \tag{3.46b}$$

- The dependent components of the sensitivity of the generalized positions right after the event:

$$Q_{\text{dep}+}\big|_{t_{\text{eve}}}^{+} = \mathsf{R}^{+}\big|_{t_{\text{eve}}}^{+} \cdot Q_{\text{dof}+}\big|_{t_{\text{eve}}}^{+} - \left(\Phi^{+}_{q_{\text{dep}+}}\big|_{t_{\text{eve}}}^{+}\right)^{-1} \Phi^{+}_{\rho}\Big|_{t_{\text{eve}}}^{+} . \tag{3.46c}$$

- The independent coordinates of the velocity sensitivities right after the event,

$$\begin{aligned} V_{\text{dof}+}\big|_{t_{\text{eve}}}^{+} &= h_q\big|_{t_{\text{eve}}}^{-} \cdot Q\big|_{t_{\text{eve}}}^{-} + h_{v_{\text{dof-}}}\big|_{t_{\text{eve}}}^{-} \cdot V_{\text{dof-}}\big|_{t_{\text{eve}}}^{-} \\ &+ \left(h_q\big|_{t_{\text{eve}}}^{-} \cdot v\big|_{t_{\text{eve}}}^{-} - \ddot{q}_{\text{dof}+}\big|_{t_{\text{eve}}}^{+} + h_{v_{\text{dof-}}}\big|_{t_{\text{eve}}}^{-} \cdot \ddot{q}_{\text{dof-}}\big|_{t_{\text{eve}}}^{-} + h_t\big|_{t_{\text{eve}}}^{-}\right) \cdot \frac{dt_{\text{eve}}}{d\rho} + h_{\rho}\big|_{t_{\text{eve}}}^{-}, \end{aligned} \tag{3.47}$$

where the Jacobians of the jump function are:

$$h_q\big|_{t_{\text{eve}}}^{-} := \frac{\partial h}{\partial q}\left(q\big|_{t_{\text{eve}}}, v_{\text{dof-}}\big|_{t_{\text{eve}}}^{-}, \rho\right) \in \mathbb{R}^{f^{+} \times n}, \qquad h_{v_{\text{dof-}}}\big|_{t_{\text{eve}}}^{-} := \frac{\partial h}{\partial v_{\text{dof-}}}\left(q\big|_{t_{\text{eve}}}, v_{\text{dof-}}\big|_{t_{\text{eve}}}^{-}, \rho\right) \in \mathbb{R}^{f^{+} \times f^{-}}.$$

$$h_t\big|_{t_{\text{eve}}}^{-} := \frac{\partial h}{\partial t}\left(q\big|_{t_{\text{eve}}}, v_{\text{dof-}}\big|_{t_{\text{eve}}}^{-}, \rho\right) \in \mathbb{R}^{f}, \qquad h_{\rho}\big|_{t_{\text{eve}}}^{-} := \frac{\partial h}{\partial \rho}\left(q\big|_{t_{\text{eve}}}, v_{\text{dof-}}\big|_{t_{\text{eve}}}^{-}, \rho\right) \in \mathbb{R}^{f \times p}.$$

- The dependent components of the velocity sensitivities right after the event,

$$V_{\text{dep}+}\big|_{t_{\text{eve}}}^{+} = -\left(\Phi^{+}_{q_{\text{dep}+}}\big|_{t_{\text{eve}}}^{+}\right)^{-1} \left(\Phi^{+}_{q_{\text{dof}+}} \cdot V_{\text{dof}+} + \left(\Phi^{+}_{q,\,q}\, v + \Phi^{+}_{t,\,q}\right) \cdot Q + \Phi^{+}_{q,\,\rho}\, v + \Phi^{+}_{t,\,\rho}\right)\Big|_{t_{\text{eve}}}^{+} . \tag{3.48}$$

Definition 3.2.4 (The generalized sensitivity jump matrix for elastic impact)**.** The jump equations (3.42)–(3.48) for constrained systems can be written compactly in matrix form as a jump of the state sensitivity matrix X at the time of the event, $X\big|_{t_{\text{eve}}}^{+} = \mathsf{S}_{\text{eve}} \cdot X\big|_{t_{\text{eve}}}^{-}$, where

$\mathsf{S}_{\mathrm{eve}}$ represents the generalized jump sensitivity matrix:

$$\begin{bmatrix} Q_{\mathrm{dep}+}|^{+}_{t_{\mathrm{eve}}} \\ Q_{\mathrm{dof}+}|^{+}_{t_{\mathrm{eve}}} \\ V_{\mathrm{dep}+}|^{+}_{t_{\mathrm{eve}}} \\ V_{\mathrm{dof}+}|^{+}_{t_{\mathrm{eve}}} \\ \Gamma|^{+}_{t_{\mathrm{eve}}} \\ Z|^{+}_{t_{\mathrm{eve}}} \end{bmatrix} = \underbrace{\begin{bmatrix} \left(Q_{\mathrm{dep}+}|^{+}_{t_{\mathrm{eve}}}\right)_{Q|^{-}_{t_{\mathrm{eve}}}} & \mathsf{0}_{(n-f)\times(n-f)} & \mathsf{0}_{(n-f)\times f} & D & \mathsf{0}_{(n-f)\times n_c} \\ \left(Q_{\mathrm{dof}+}|^{+}_{t_{\mathrm{eve}}}\right)_{Q|^{-}_{t_{\mathrm{eve}}}} & \mathsf{0}_{f\times(n-f)} & \mathsf{0}_{f\times f} & \mathsf{0}_{f\times p} & \mathsf{0}_{f\times n_c} \\ \left(V_{\mathrm{dep}+}|^{+}_{t_{\mathrm{eve}}}\right)_{Q|^{-}_{t_{\mathrm{eve}}}} & \mathsf{0}_{(n-f)\times(n-f)} & \left(V_{\mathrm{dep}+}|^{+}_{t_{\mathrm{eve}}}\right)_{V_{\mathrm{dof}+}|^{-}_{t_{\mathrm{eve}}}} & K & \mathsf{0}_{(n-f)\times n_c} \\ \left(V_{\mathrm{dof}+}|^{+}_{t_{\mathrm{eve}}}\right)_{Q|^{-}_{t_{\mathrm{eve}}}} & \mathsf{0}_{f\times(n-f)} & h_v|^{-}_{t_{\mathrm{eve}}} & h_\rho|^{-}_{t_{\mathrm{eve}}} & \mathsf{0}_{f\times n_c} \\ \mathsf{0}_{p\times n} & \mathsf{0}_{p\times(n-f)} & \mathsf{0}_{p\times f} & \mathsf{I}_{p\times p} & \mathsf{0}_{p\times n_c} \\ \left(Z|^{+}_{t_{\mathrm{eve}}}\right)_{Q|^{-}_{t_{\mathrm{eve}}}} & \mathsf{0}_{n_c\times(n-f)} & \mathsf{0}_{n_c\times f} & \mathsf{0}_{n_c\times p} & \mathsf{I}_{n_c\times n_c} \end{bmatrix}}_{\mathsf{S}_{\mathrm{eve}}} \cdot \begin{bmatrix} Q_{\mathrm{dep}+}|^{-}_{t_{\mathrm{eve}}} \\ Q_{\mathrm{dof}+}|^{-}_{t_{\mathrm{eve}}} \\ V_{\mathrm{dep}+}|^{-}_{t_{\mathrm{eve}}} \\ V_{\mathrm{dof}+}|^{-}_{t_{\mathrm{eve}}} \\ \Gamma|^{-}_{t_{\mathrm{eve}}} \\ Z|^{-}_{t_{\mathrm{eve}}} \end{bmatrix} \tag{3.49}$$

The Jacobians of the jump equations with respect to the sensitivity state before the time of event are:

$$\left(Q_{\mathrm{dof}+}|^{+}_{t_{\mathrm{eve}}}\right)_{Q|^{-}_{t_{\mathrm{eve}}}} = \mathsf{P}^{+}_{\mathrm{dof}+}\left(\mathsf{I}_{\mathrm{n\times n}} - \left(\mathrm{v}|^{+}_{\mathrm{t_{eve}}} - \mathrm{v}|^{-}_{\mathrm{t_{eve}}}\right) \cdot \left(\frac{\mathrm{dt_{eve}}}{\mathrm{d}\rho}\right)_{\mathrm{Q}|^{-}_{\mathrm{t_{eve}}}}\right)(\mathsf{P}^{-})^{\mathrm{T}} \in \mathbb{R}^{f\times n}, \tag{3.50}$$

with

$$\left(\frac{dt_{\mathrm{eve}}}{d\rho}\right)_{Q|^{-}_{t_{\mathrm{eve}}}} = -\frac{\dfrac{dr}{dq}\left(q|_{t_{\mathrm{eve}}}\right)}{\dfrac{dr}{dq}\left(q|_{t_{\mathrm{eve}}}\right)\cdot v|^{-}_{t_{\mathrm{eve}}}} \in \mathbb{R}^{1\times n}. \tag{3.51}$$

It follows that:

$$\left(Q_{\mathrm{dep}+}|^{+}_{t_{\mathrm{eve}}}\right)_{Q|^{-}_{t_{\mathrm{eve}}}} = \mathsf{R}^{+}|^{+}_{t_{\mathrm{eve}}} \cdot \left(Q_{\mathrm{dof}+}|^{+}_{t_{\mathrm{eve}}}\right)_{Q|^{-}_{t_{\mathrm{eve}}}} \in \mathbb{R}^{(n-f)\times n}, \tag{3.52}$$

and

$$\begin{aligned}&\left(V_{\text{dof+}}\big|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}} = \\ &\left(h_q\big|_{t_{\text{eve}}}^{-} + \left(h_q\big|_{t_{\text{eve}}}^{-} \cdot v\big|_{t_{\text{eve}}}^{-} - \ddot{q}_{\text{dof+}}\big|_{t_{\text{eve}}}^{+} + h_{v_{\text{dof-}}}\big|_{t_{\text{eve}}}^{-} \cdot \ddot{q}_{\text{dof-}}\big|_{t_{\text{eve}}}^{-} + h_t\big|_{t_{\text{eve}}}^{-}\right) \cdot \left(\frac{dt_{\text{eve}}}{d\rho}\right)_{Q|_{t_{\text{eve}}}^{-}}\right) \cdot (\mathsf{P}^{-})^{\mathrm{T}} \in \mathbb{R}^{f\times n}.\end{aligned} \tag{3.53}$$

Rewriting (3.48) as:

$$\left(V_{\text{dep+}}\big|_{t_{\text{eve}}}^{+}\right) = \left(\mathsf{R}^{+} \cdot V_{\text{dof+}} + \overline{\mathsf{R}}^{+} \cdot Q + C\right)\Big|_{t_{\text{eve}}}^{+} \in \mathbb{R}^{(n-f)\times p} \tag{3.54}$$

or, equivalently, as:

$$\begin{aligned}\left(V_{\text{dep+}}\big|_{t_{\text{eve}}}^{+}\right) &= \left(\mathsf{R}^{+} \cdot V_{\text{dof+}} + \overline{\mathsf{R}}^{+} \cdot (\mathsf{P}^{-})^{\mathrm{T}} \cdot \begin{bmatrix} Q_{\text{dep+}}\big|_{t_{\text{eve}}}^{-} \\ Q_{\text{dof+}}\big|_{t_{\text{eve}}}^{-} \end{bmatrix} + C\right)\Bigg|_{t_{\text{eve}}}^{+}, \\ \overline{\mathsf{R}}^{+}\big|_{t_{\text{eve}}}^{+} &= -\left(\Phi^{+}_{q_{\text{dep+}}}\right)^{-1}\left(\Phi^{+}_{q,\,q}\, v + \Phi^{+}_{t,\,q}\right)\Big|_{t_{\text{eve}}}^{+}, \\ C &= -\left(\Phi^{+}_{q_{\text{dep+}}}\right)^{-1}\left(\Phi^{+}_{q,\,\rho}\, v + \Phi^{+}_{t,\,\rho}\right)\Big|_{t_{\text{eve}}}^{+} \in \mathbb{R}^{(n-f)\times p},\end{aligned} \tag{3.55}$$

we find the following expressions for the Jacobians:

$$\begin{aligned}\left(V_{\text{dep+}}\big|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}} &= \mathsf{R}^{+}\big|_{t_{\text{eve}}}^{+} \cdot \left(V_{\text{dof+}}\big|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}} + \overline{\mathsf{R}}^{+}\big|_{t_{\text{eve}}}^{+} \cdot (\mathsf{P}^{-})^{\mathrm{T}} \quad \mathbb{R}^{(n-f)\times n}, \\ \left(V_{\text{dep+}}\big|_{t_{\text{eve}}}^{+}\right)_{V_{\text{dof+}}|_{t_{\text{eve}}}^{-}} &= \mathsf{R}^{+}\big|_{t_{\text{eve}}}^{+} \cdot h_v\big|_{t_{\text{eve}}}^{-}.\end{aligned} \tag{3.56}$$

The expressions for D and K in (3.49) are:

$$
\begin{aligned}
D &= -\left(\Phi^+_{q_{\text{dep}+}}\right)^{-1} \Phi^+_{\rho}\Big|^{+}_{t_{\text{eve}}} \in \mathbb{R}^{(n-f)\times p},\\
K &= \left(C + \mathsf{R}^+ \cdot h_{\rho}\big|^{-}_{t_{\text{eve}}} + \overline{\mathsf{R}}^+ \cdot (\mathsf{P}^-)^{\mathrm{T}} \cdot \begin{bmatrix} D \\ \mathsf{0}_{f\times p} \end{bmatrix} \right)\Bigg|^{+}_{t_{\text{eve}}} \in \mathbb{R}^{(n-f)\times p}.
\end{aligned}
\tag{3.57}
$$

Definition 3.2.5 (The generalized sensitivity jump matrix for inelastic impact with a sudden change of constraints)**.** Consider the event consisting of an inelastic collision and a sudden change of constraints (3.44). The jump in the velocity sensitivity for constrained systems due to impulsive forces, presented in [64], is determined as follows:

$$
\begin{aligned}
\begin{bmatrix} V\big|^{+}_{t_{\text{eve}}} \\ \delta\Lambda \end{bmatrix} = &- \begin{bmatrix} \mathsf{M} & {\Phi^{+}_{q}}^{\mathrm{T}} \\ \Phi^{+}_{q} & \mathsf{0} \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{M}_q \cdot \left(v\big|^{+}_{t_{\text{eve}}} - v\big|^{-}_{t_{\text{eve}}}\right) + {\Phi^{+}_{q,\,q}}^{\mathrm{T}} \cdot \delta\lambda \\ \Phi^{+}_{q,\,q} \cdot v\big|^{+}_{t_{\text{eve}}} \end{bmatrix} \cdot Q\big|^{+}_{t_{\text{eve}}} \\
&+ \begin{bmatrix} \mathsf{M} & {\Phi^{+}_{q}}^{\mathrm{T}} \\ \Phi^{+}_{q} & \mathsf{0} \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{M} \\ \mathsf{0} \end{bmatrix} \cdot V\big|^{-}_{t_{\text{eve}}} - \begin{bmatrix} \mathsf{M} & {\Phi^{+}_{q}}^{\mathrm{T}} \\ \Phi^{+}_{q} & \mathsf{0} \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{M}_{\rho} \cdot v\big|^{+}_{t_{\text{eve}}} + {\Phi^{+}_{q,\,\rho}}^{\mathrm{T}} \cdot \delta\lambda \\ \Phi^{+}_{q,\,\rho} \cdot v\big|^{+}_{t_{\text{eve}}} + \Phi^{+}_{t,\,\rho} \cdot v\big|^{-}_{t_{\text{eve}}} \end{bmatrix} \\
&- \begin{bmatrix} \mathsf{M} & {\Phi^{+}_{q}}^{\mathrm{T}} \\ \Phi^{+}_{q} & \mathsf{0} \end{bmatrix}^{-1} \begin{bmatrix} \mathsf{0} \\ \Phi^{+}_{t,\,q} \cdot v\big|^{-}_{t_{\text{eve}}} + \Phi^{+}_{t,\,v} \cdot v\big|^{-}_{t_{\text{eve}}} \end{bmatrix},
\end{aligned}
\tag{3.58}
$$

which simplifies to:

$$\begin{bmatrix} V|_{t_{\text{eve}}}^{+} \\ \\ \delta\Lambda \end{bmatrix} = f_q^{\text{DAE-imp}} \cdot Q|_{t_{\text{eve}}}^{+} + f_{v|_{t_{\text{eve}}}^{-}}^{\text{DAE-imp}} \cdot V|_{t_{\text{eve}}}^{-} + f_\rho^{\text{DAE-imp}} + f_t^{\text{DAE-imp}}. \tag{3.59}$$

Thus, the jump the velocity state variables at the time of event is

$$V|_{t_{\text{eve}}}^{+} = f_q^{\text{DAE-imp-}v}|_{t_{\text{eve}}}^{+}\, Q|_{t_{\text{eve}}}^{+} + f_v^{\text{DAE-imp-}v}|_{t_{\text{eve}}}^{+}\, V|_{t_{\text{eve}}}^{+} + f_\rho^{\text{DAE-imp-}v}|_{t_{\text{eve}}}^{+}, \tag{3.60}$$

and the jump in the sensitivity of the Lagrange multipliers from $\Lambda|_{t_{\text{eve}}}^{-} \to \Lambda|_{t_{\text{eve}}}^{+}$ is:

$$\Lambda|_{t_{\text{eve}}}^{+} = \Lambda|_{t_{\text{eve}}}^{-} + f_q^{\text{DAE-imp-}\mu}|_{t_{\text{eve}}}^{+}\, Q|_{t_{\text{eve}}}^{+} + f_v^{\text{DAE-imp-}\mu}|_{t_{\text{eve}}}^{+}\, V|_{t_{\text{eve}}}^{+} + f_\rho^{\text{DAE-imp-}\mu}|_{t_{\text{eve}}}^{+}. \tag{3.61}$$

The corresponding sensitivity jump matrix (3.49) is:

$$\begin{bmatrix} Q_{\text{dep}+}|_{t_{\text{eve}}}^{+} \\ Q_{\text{dof}+}|_{t_{\text{eve}}}^{+} \\ V|_{t_{\text{eve}}}^{+} \\ \Lambda|_{t_{\text{eve}}}^{+} \\ \Gamma|_{t_{\text{eve}}}^{+} \\ Z|_{t_{\text{eve}}}^{+} \end{bmatrix} = \underbrace{\begin{bmatrix} \left(Q_{\text{dep}+}|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}} & \mathsf{0}_{(n-f)\times n} & \mathsf{0}_{(n-f)\times m} & D & \mathsf{0}_{(n-f)\times n_c} \\ \left(Q_{\text{dof}+}|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}} & \mathsf{0}_{f\times n} & \mathsf{0}_{f\times m} & \mathsf{0}_{f\times p} & \mathsf{0}_{f\times n_c} \\ f_q^{\text{DAE-imp-}v}|_{t_{\text{eve}}}^{+} & f_v^{\text{DAE-imp-}v}|_{t_{\text{eve}}}^{+} & \mathsf{0}_{n\times m} & f_\rho^{\text{DAE-imp-}v}|_{t_{\text{eve}}}^{+} & \mathsf{0}_{n\times nc} \\ f_q^{\text{DAE-imp-}\mu}|_{t_{\text{eve}}}^{+} & f_v^{\text{DAE-imp-}\mu}|_{t_{\text{eve}}}^{+} & \mathsf{0}_{m\times m} & f_\rho^{\text{DAE-imp-}\mu}|_{t_{\text{eve}}}^{+} & \mathsf{0}_{m\times nc} \\ \mathsf{0}_{p\times n} & \mathsf{0}_{p\times n} & \mathsf{0}_{p\times m} & \mathsf{I}_{p\times p} & \mathsf{0}_{p\times n_c} \\ \left(Z|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}} & \mathsf{0}_{n_c\times n} & \mathsf{0}_{n_c\times m} & \mathsf{0}_{n_c\times p} & \mathsf{I}_{n_c\times n_c} \end{bmatrix}}_{\mathsf{S}_{\text{eve}}} \cdot \begin{bmatrix} Q_{\text{dep}+}|_{t_{\text{eve}}}^{-} \\ Q_{\text{dof}+}|_{t_{\text{eve}}}^{-} \\ V|_{t_{\text{eve}}}^{-} \\ \Lambda|_{t_{\text{eve}}}^{-} \\ \Gamma|_{t_{\text{eve}}}^{-} \\ Z|_{t_{\text{eve}}}^{-} \end{bmatrix} \tag{3.62}$$

3.2.5 Adjoint sensitivity analysis for hybrid constrained dynamical systems

Definition 3.2.6 (Jump in adjoint sensitivity for constrained systems with elastic impact)**.** The transpose of the direct sensitivity jump matrix $\mathsf{S}_{\text{eve}}^{\mathrm{T}}$ (3.28) associated with an elastic impact (3.49) is:

$$\mathsf{S}_{\text{eve}}^{\mathrm{T}} =$$

$$\begin{bmatrix} \left(Q_{\text{dep}+}|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} & \left(Q_{\text{dof}+}|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} & \left(V_{\text{dep}+}|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} & \left(V_{\text{dof}+}|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} & \mathsf{0}_{n\times p} & \left(Z|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} \\ \mathsf{0}_{(n-f)\times(n-f)} & \mathsf{0}_{(n-f)\times f} & \mathsf{0}_{(n-f)\times(n-f)} & \mathsf{0}_{(n-f)\times f} & 0_{(n-f)\times p} & 0_{(-n-f)\times n_c} \\ \mathsf{0}_{f\times(n-f)} & \mathsf{0}_{f\times f} & \left(V_{\text{dep}+}|_{t_{\text{eve}}}^{+}\right)_{V_{\text{dof}+}|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} & \left[h_v|_{t_{\text{eve}}}^{-}\right]^{\mathrm{T}} & 0_{f\times p} & 0_{f\times p} \\ D^{\mathrm{T}} & \mathsf{0}_{p\times f} & K^{\mathrm{T}} & \left[h_\rho|_{t_{\text{eve}}}^{-}\right]^{\mathrm{T}} & \mathsf{I}_{p\times p} & 0_{p\times n_c} \\ 0_{n_c\times(n-f)} & 0_{n_c\times f} & 0_{n_c\times(n-f)} & \mathsf{0}_{n_c\times f} & 0_{n_c\times p} & \mathsf{I}_{n_c\times n_c} \end{bmatrix} \tag{3.63}$$

From the adjoint sensitivity equation (3.28) the jumps in adjoint variables for ODE systems with constraints undergoing an elastic impact are:

$$
\begin{aligned}
\lambda^{Q}\big|_{t_{\text{eve}}}^{-} &= \left[\left(Q_{\text{dep}+}\big|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} \quad \left(Q_{\text{dof}+}\big|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}}\right] \cdot \lambda^{Q}\big|_{t_{\text{eve}}}^{+} + \\
&\quad \left[\left(V_{\text{dep}+}\big|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} \quad \left(V_{\text{dof}+}\big|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}}\right] \cdot \lambda^{V}\big|_{t_{\text{eve}}}^{+} + \left(Z\big|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} \cdot \lambda^{Z}\big|_{t_{\text{eve}}}^{+} \\
\lambda^{V}\big|_{t_{\text{eve}}}^{-} &= \begin{bmatrix} \mathsf{0}_{(n-f)\times f} & \mathsf{0}_{(n-f)\times f} \\ \left(V_{\text{dep}+}\big|_{t_{\text{eve}}}^{+}\right)_{V_{\text{dof}+}|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} & \left[h_{v}\big|_{t_{\text{eve}}}^{-}\right]^{\mathrm{T}} \end{bmatrix} \cdot \lambda^{V}\big|_{t_{\text{eve}}}^{+} \\
\lambda^{\Gamma}\big|_{t_{\text{eve}}}^{-} &= \begin{bmatrix} D^{\mathrm{T}} & \mathsf{0}_{p\times f} \end{bmatrix} \cdot \lambda^{Q}\big|_{t_{\text{eve}}}^{+} + \begin{bmatrix} K^{\mathrm{T}} & h_{\rho}\big|_{t_{\text{eve}}}^{-}{}^{\mathrm{T}} \end{bmatrix} \cdot \lambda^{V}\big|_{t_{\text{eve}}}^{+} + \lambda^{\Gamma}\big|_{t_{\text{eve}}}^{+} \\
\lambda^{Z}\big|_{t_{\text{eve}}}^{-} &= \lambda^{Z}\big|_{t_{\text{eve}}}^{+}
\end{aligned}
\tag{3.64}
$$

Definition 3.2.7 (Jump in adjoint sensitivity for constrained systems with inelastic impact and a sudden change of constraints)**.** The transpose of the direct sensitivity jump matrix $\mathsf{S}_{\text{eve}}^{\mathrm{T}}$ (3.28) associated with (3.62) is:

$$
\mathsf{S}_{\text{eve}}^{\mathrm{T}} =
$$

$$
\begin{bmatrix}
\left(Q_{\text{dep}+}\big|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} & \left(Q_{\text{dof}+}\big|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} & \left[f_{q}^{\text{DAE-imp-}v}\big|_{t_{\text{eve}}}^{+}\right]^{\mathrm{T}} & \left[f_{q}^{\text{DAE-imp-}\mu}\big|_{t_{\text{eve}}}^{+}\right]^{\mathrm{T}} & \mathsf{0}_{n\times p} & \left(Z\big|_{t_{\text{eve}}}^{+}\right)_{Q|_{t_{\text{eve}}}^{-}}^{\mathrm{T}} \\
\mathsf{0}_{n\times(n-f)} & \mathsf{0}_{n\times f} & \left[f_{v}^{\text{DAE-imp-}v}\big|_{t_{\text{eve}}}^{+}\right]^{\mathrm{T}} & \left[f_{v}^{\text{DAE-imp-}\mu}\big|_{t_{\text{eve}}}^{+}\right]^{\mathrm{T}} & \mathsf{0}_{n\times(p)} & \mathsf{0}_{n\times(n_c)} \\
\mathsf{0}_{m\times(n-f)} & \mathsf{0}_{m\times f} & \mathsf{0}_{m\times n} & \mathsf{0}_{m\times m} & \mathsf{0}_{m\times(p)} & \mathsf{0}_{m\times(n_c)} \\
D^{\mathrm{T}} & \mathsf{0}_{p\times f} & \left[f_{\rho}^{\text{DAE-imp-}v}\big|_{t_{\text{eve}}}^{+}\right]^{\mathrm{T}} & \left[f_{\rho}^{\text{DAE-imp-}\mu}\big|_{t_{\text{eve}}}^{+}\right]^{\mathrm{T}} & \mathsf{I}_{p\times p} & 0_{p\times n_c} \\
\mathsf{0}_{n_c\times(n-f)} & \mathsf{0}_{n_c\times f} & \mathsf{0}_{n_c\times n} & \mathsf{0}_{n_c\times m} & \mathsf{0}_{n_c\times(p)} & \mathsf{I}_{n_c\times n_c}
\end{bmatrix}
\tag{3.65}
$$

Since the adjoints of the algebraic Lagrange variables are zero (Remark 3.2.1), the adjoint sensitivity equations (3.28) provide the jump equations for adjoint variables at the time of event:

$$
\begin{aligned}
\lambda^{Q}|_{t_{\mathrm{eve}}}^{-} &= \left[\left(Q_{\mathrm{dep+}}|_{t_{\mathrm{eve}}}^{+}\right)_{Q|_{t_{\mathrm{eve}}}^{-}}^{\mathrm{T}} \quad \left(Q_{\mathrm{dof+}}|_{t_{\mathrm{eve}}}^{+}\right)_{Q|_{t_{\mathrm{eve}}}^{-}} \right] \cdot \lambda^{Q}|_{t_{\mathrm{eve}}}^{+} + \\
&\qquad \left[f_{q}^{\text{DAE-imp-}v}|_{t_{\mathrm{eve}}}^{+}\right]^{\mathrm{T}} \cdot \lambda^{V}|_{t_{\mathrm{eve}}}^{+} + \left(Z|_{t_{\mathrm{eve}}}^{+}\right)_{Q|_{t_{\mathrm{eve}}}^{-}}^{\mathrm{T}} \cdot \lambda^{Z}|_{t_{\mathrm{eve}}}^{+}, \\
\lambda^{V}|_{t_{\mathrm{eve}}}^{-} &= \left[f_{v}^{\text{DAE-imp-}v}|_{t_{\mathrm{eve}}}^{+}\right]^{\mathrm{T}} \cdot \lambda^{V}|_{t_{\mathrm{eve}}}^{+}, \\
\lambda^{\Gamma}|_{t_{\mathrm{eve}}}^{-} &= \begin{bmatrix} D^{\mathrm{T}} & \mathsf{0}_{p\times f} \end{bmatrix} \cdot \lambda^{Q}|_{t_{\mathrm{eve}}}^{+} + \left[f_{\rho}^{\text{DAE-imp-}v}|_{t_{\mathrm{eve}}}^{+}\right]^{\mathrm{T}} \cdot \lambda^{V}|_{t_{\mathrm{eve}}}^{+} + \lambda^{\Gamma}|_{t_{\mathrm{eve}}}^{+}, \\
\lambda^{Z}|_{t_{\mathrm{eve}}}^{-} &= \lambda^{Z}|_{t_{\mathrm{eve}}}^{+}.
\end{aligned}
\tag{3.66}
$$

Remark (Sensitivities of the cost function)*.* Once the evolution of the sensitivities of the direct or adjoint sensitivities are computed, the sensitivity of the cost function with respect to parameters $d\,\psi/d\,\rho$ is obtained from equations (3.18) and (3.21). Note that the evolution of the direct and adjoint sensitivities involve is piecewise continuous in time, with jumps occurring at each event.

3.3 Case study: sensitivity analysis of a five-bar mechanism

A five-bar mechanism is used as a case study to apply the presented mathematical framework. The presentation of the mechanism and the evolution of the position and velocity trajectories of the bottom point of the mechanism are provided in Appendix C.

The trajectory of the quadrature variables $z(t) = \int_{t_0}^{t} \dot{y}_2(\tau)\, \mathrm{d}\tau$ and $z(t) = \int_{t_0}^{t} \ddot{y}_2\, \mathrm{d}\tau$ of the five-bar mechanism are shown in Fig. 2.3a and Fig. 2.3b, respectively. Their respective sensitivities are presented in Fig. 3.1 and Fig. 3.2.

The direct sensitivity is represented by the continuous line, while the central finite difference sensitivity is represented by the dashed line. Both solutions were solved forward in time. The adjoint sensitivity is presented as well, and was solved backwards in time. As presented in the previous chapter, the direct differentiation method to compute the sensitivity of the cost function with discontinuities in the velocity state variables of the mechanism is validated. The validation comes to the fact that the trajectories of the sensitivity of the quadrature variable $Z(\, t,\, q,\, v,\, \rho\,)$ exactly matches the trajectory of numerical sensitivity computed with a finite difference method. One main conclusion of our previous chapter was to state that our proposed direct sensitivity method in computing the sensitivity of the cost function with discontinuities in the velocity state variables was more robust than the numerical method. Indeed, the direct method accurately determines the jump in the sensitivities and their trajectories. This after each event, without any delta-like jumps in magnitude $1/\varepsilon$ that occurs in the numerical method at each time of event. This validated direct sensitivity method is now compared to the proposed adjoint method in computing the sensitivity of the cost function with discontinuities in the velocity state variables. The results presented in Fig. 3.1 and Fig. 3.2 show that the adjoint and direct method exactly converge to the same sensitivity cost number with a difference of less than 0.01 %.

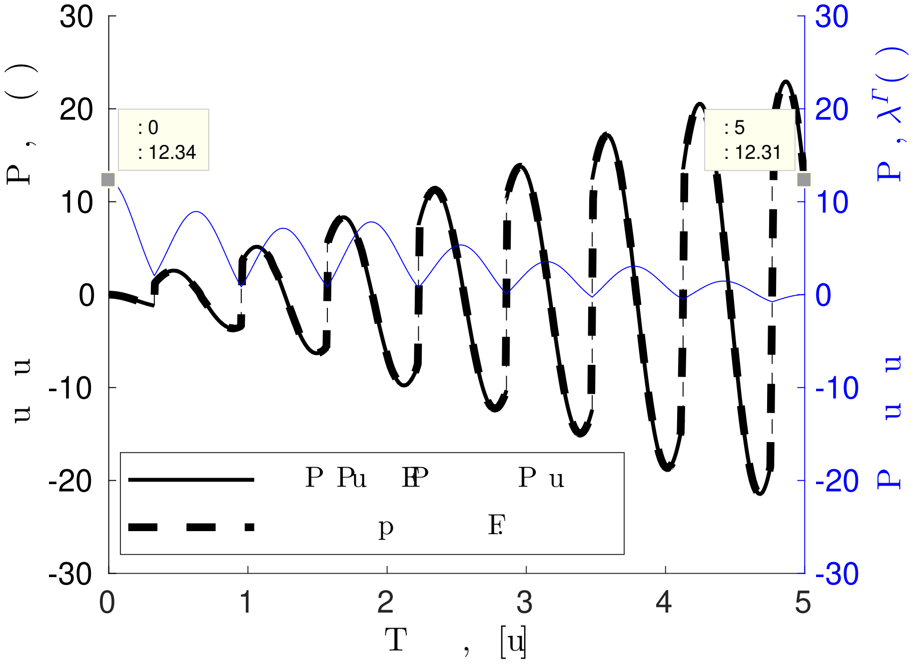


Figure 3.1: Sensitivity analysis of the five-bar mechanism with $z(t) = \int_{t_0}^{t} \dot{y}_2(\tau)\ \mathrm{d}\tau$.

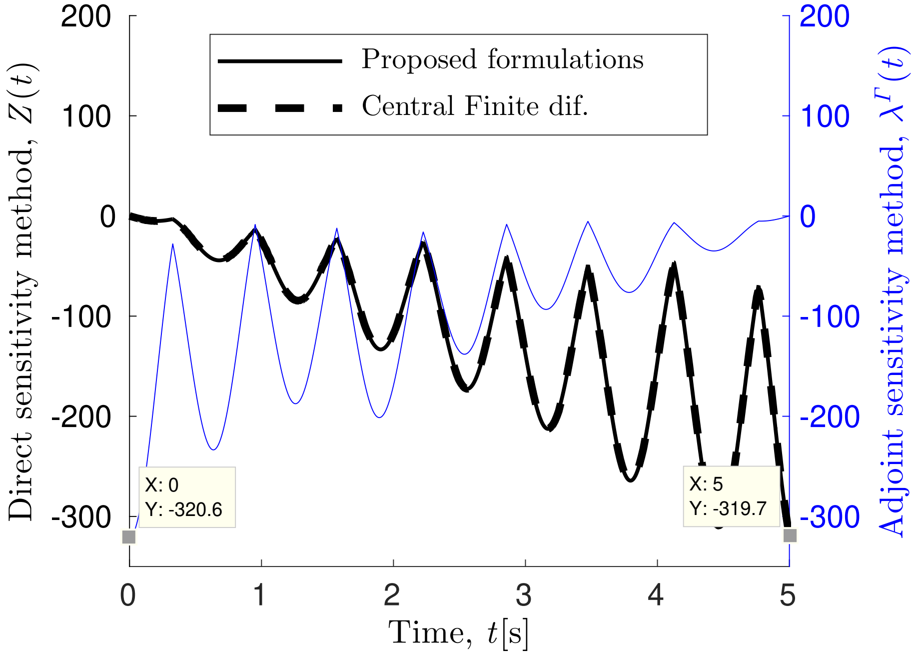


Figure 3.2: Sensitivity analysis of the five-bar mechanism with $z(t) = \int_{t_0}^{t} \ddot{y}_2\ \mathrm{d}\tau$.

This convergence in both methods validates the adjoint sensitivity method in computing the sensitivity of the cost function with discontinuities in the trajectories. Note that $z(t) = \int_{t_0}^{t} \ddot{y}_2(\tau)\ \mathrm{d}\tau$ does not completely match the trajectory of the velocity of point 2 in Fig. C.2b. Indeed, the point2's velocity jumps at the time of event, while the quadrature variable does not. The quadrature variable evaluates the integral of the acceleration of point 2 only.

The same analysis is provided with a quadrature variable $z(t) = \int_{t_0}^{t} \ddot{y}_2(\tau)^2 + \dot{y}_2(\tau)^2\ \mathrm{d}\tau$. the evolution of the quadrature variable and its sensitivity are presented in in Fig. 3.3 and Fig. 3.4, respectively. The final data points for each method show that the adjoint and the direct method in computing sensitivity of the quadrature variable converge to the same sensitivity cost number with a difference of less than 0.01 %.

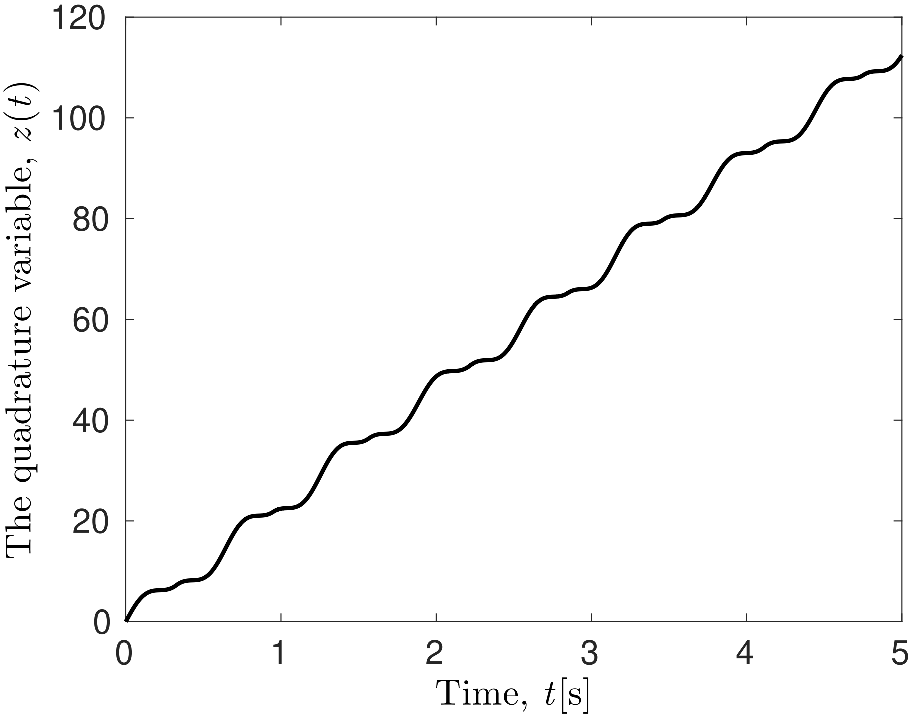


Figure 3.3: The sensitivity of the quadrature variable.

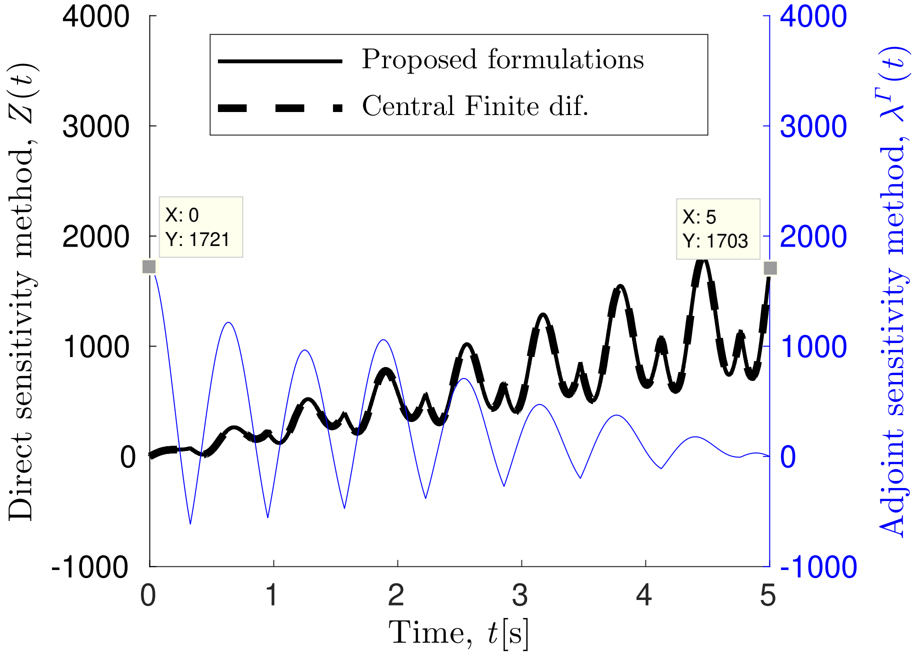


Figure 3.4: Sensitivity analysis of the five-bar mechanism with $z(t) = \int_{t_0}^{t} \ddot{y}_2(\tau)^2 + \dot{y}_2(\tau)^2 \, \mathrm{d}\tau$.

Chapter 4

Conclusion

This dissertation targets the needs of a large audience as it provides a unified methodology and the associated mathematical tools that advance the state-of-the-art in the sensitivity analysis field. It provides a complete mathematical framework needed to compute the sensitivities of model states and of general cost functionals with respect to model parameters for both, unconstrained and constrained hybrid mechanical systems.

Jump conditions for sensitivity variables and general cost functionals are established for both, the ordinary and the differential algebraic equations cases. These jump conditions specify the values of the sensitivities right after the event, given their value right before the event, and the characteristics of the impact. The impacts can be characterized as a sudden jump in the velocity state variables caused by impulsive forces, changes in the equations of motion, or changes in the kinematic constraints. The dissertation provides new graphical proofs of the jumps in sensitivities at the time of an event, which helps to better understand the conditions for the jump in the sensitivities.

A five-bar mechanism with non-smooth contacts is used as a case study. The analytical sensitivities obtained by the proposed methodology are validated against numerical sensitivities computed by central finite differences. The results of the case study show that the analytical sensitivity is more robust than the numerical method, as it correctly calculates the sensitivities of piecewise trajectories without any delta-like jumps.

The mathematical framework is also applied on the Iltis vehicle. The analytical sensitivities obtained are also validated against numerical sensitivities computed by central finite differences. This study clearly shows that the necessary used of an analytically analysis when solving the sensitivities of complex multibody systems. The finite difference cannot be trustful if the mechanical system has forward non-smooth trajectories.

Many formalisms to model constrained mechanical systems exist. However, this research emphasizes the use of the penalty formulation. This formulation has the advantage that it incorporates the kinematic constraints inside the equation of motion. Thus, it avoids any discontinuities in the velocity trajectories due to changes in the set of constraints at the time of event. This formalism is in the form of an ODE, which considerably eases the numerical integration by avoiding algebraic variables. Also, this formalism works well for systems with redundant constraints and for systems that encounter a kinematic bifurcation. Although there exists a multitude of formalisms and methodology approaches for modeling a constrained mechanical system, most of them are ODE- or DAE-based formalisms. For this reason, this study also provides the DAE rank 1 and 3 for modeling constrained mechanical systems.

One of the most significant accomplishments presented in this dissertation is a unified mathematical framework for performing the direct and the adjoint sensitivity analysis for general hybrid systems associated with general cost functions. The mathematical framework handles the non-smoothness of the forward trajectories, while performing adjoint sensitivity analysis. To handle such situations, the mathematical framework computes the jump sensitivity matrix of the direct sensitivities, which is found by computing the Jacobian of the jump conditions with respect to sensitivities right before the event. The main idea was then to obtain the transpose of the jump sensitivity matrix to compute the jump conditions for the the adjoint sensitivities.

Furthermore, in this framework, the sensitivity matrix of cost functions with respect to parameters for general hybrid ODE systems was obtained. Such matrix is a key result for design analysis, as it provides the parameters that affect the given cost functions the most. Such results could be applied to gradient based algorithms, control optimization, implicit time integration methods, deep learning, etc.

Current efforts focus on applying the hybrid system sensitivity analysis methodology to robotics, where sensitivities of the performance of a robotic system with respect to changes in the system configuration under non-smooth impact conditions are a topic of great interest. Ongoing work extends the current framework to perform adjoint sensitivity analysis of other types of hybrid mechanical systems.

Future Work

The mathematical framework developed in this research can open the gate to many other research possibilities and can help address research aspects, such as:

- Dynamic modeling, TLM, and adjoint sensitivity analysis of a passive bipedal robot. When walking, such a robot exhibits discontinuities in velocities due to impacts and changes of mechanical constraints caused by the switch of the supported foot. Performing the sensitivity analysis for such a system would allow the investigation of the effect of the variation of each parameter on the dynamics of the walking robot.

- Sensitivity analysis for actuating signals. The presented mathematical framework works for cost functions with dependency on an extended function. This methodology can help identify the effect of the variation of the control signal onto the dynamics of the system.

- Terramechanics and ground contact simulation. Off-road vehicle simulation and walking motion on soft ground are excellent case studies of hybrid multibody dynamic systems where the framework developed in this dissertation can be employed to study the sensitivity analysis of such systems with respect to various parameters.

- Grazing, infinite and multi events. Many mechanisms deal with multitude of instantaneous events that leads systems to be over-constrained. One of the impact can be tangential to the event function which leads to grazing phenomena. Events can also happen infinitely as a bouncing ball which yields to zeno phenomena.

- Machine learning, reinforcement learning. The use of adjoint variables is widely used in such topics. It would be of interest to explore if the jumps conditions developed in this research can help better understand machine learning algorithms.
- Integration method. When performing sensitivity analysis in this research, the focus was on the evolution of the right hand-side and cost functions. It is known that the state variables depend on the evolution of the right hand-side since they are obtained from these terms by integration. It could be of interest to explore how a variation in the parameters of an integrator affects the time step and thus the calculated new states.

Appendices

Appendix A

Terminology used in Section 2.3

In Eqs. Eq. (2.67) the terms $\overline{\mathsf{F}}_q$, $\overline{\mathsf{F}}_{\dot q}$, $\overline{\mathsf{F}}_\rho$, $\overline{\mathsf{M}}_q\ddot q$, and $\overline{\mathsf{M}}_\rho\ddot q$ are given by the following expressions:

$$
\begin{aligned}
&\overline{\mathsf{F}}_q = \mathsf{F}_q - \Phi_{qq}^{\mathrm{T}}\alpha\left(\dot\Phi_q\dot q\dot\Phi_t + 2\,\xi\,\omega\,\dot\Phi + \omega^2\Phi\right) - \\
&\Phi_q^{\mathrm{T}}\alpha\left(\left(\dot\Phi_q\dot q\right)_q + \left(\dot\Phi_t\right)_q + 2\xi\omega\left(\Phi_{qq}\dot q + \Phi_{tq}\right) + \omega^2\Phi_q\right), && \text{(A.1)}\\
&\overline{\mathsf{F}}_{\dot q} = \mathsf{F}_{\dot q} - \Phi_q^{\mathrm{T}}\alpha\left(\Phi_{qq}\dot q + \dot\Phi_q + \Phi_{tq} + 2\,\xi\,\omega\,\Phi_q\right), && \text{(A.2)}\\
&\overline{\mathsf{F}}_\rho = \mathsf{F}_\rho - \Phi_{q\rho}^{\mathrm{T}}\alpha\left(\dot\Phi_q\dot q + \dot\Phi_t + 2\,\xi\,\omega\,\dot\Phi + \omega^2\Phi\right) - \\
&\Phi_q^{\mathrm{T}}\alpha\left(\left(\dot\Phi_q\dot q\right)_\rho + \dot\Phi_{t\rho} + 2\,\xi\,\omega\,\dot\Phi_\rho + \omega^2\Phi_\rho\right), && \text{(A.3)}\\
&\overline{\mathsf{M}}_q\ddot q = \mathsf{M}_q\ddot q + \Phi_{qq}^{\mathrm{T}}\left(\alpha\Phi_q\ddot q\right) + \Phi_q^{\mathrm{T}}\alpha\left(\Phi_{qq}\ddot q\right), && \text{(A.4)}\\
&\overline{\mathsf{M}}_\rho\ddot q = \mathsf{M}_\rho\ddot q + \Phi_{q\rho}^{\mathrm{T}}\left(\alpha\Phi_q\ddot q\right) + \Phi_q^{\mathrm{T}}\alpha\left(\Phi_{q\rho}\ddot q\right). && \text{(A.5)}
\end{aligned}
$$

In Eq. 2.68 the terms $\mu_{\dot v}^*$, μ_v^*, μ_q^* , and μ_ρ^* are given by the following expressions:

$$\mu_{\dot{v}}^{*} = \alpha \Phi_{q} \tag{A.6}$$

$$\mu_{v}^{*} = \alpha \left[\Phi_{q,q} v + \dot{\Phi}_{q} + \Phi_{tq} + 2\xi\omega\Phi_{q} \right] \tag{A.7}$$

$$\begin{aligned} \mu_{q}^{*} = \alpha \Big[& \Phi_{q,q}\dot{v} + \left(\dot{\Phi}_{q}\right)_{q} v + \left(\Phi_{t}\right)_{q} \\ & +2\xi\omega \left(\Phi_{q,q} v + \Phi_{tq}\right) + \omega^{2}\Phi_{q} \Big] \end{aligned} \tag{A.8}$$

$$\begin{aligned} \mu_{\rho}^{*} = \alpha \Big[& \Phi_{q\rho}\dot{v} + \left(\dot{\Phi}_{q}\right)_{\rho} v + \left(\dot{\Phi}_{t}\right)_{\rho} \\ & +2\xi\omega \left(\Phi_{q\rho} v + \Phi_{t\rho}\right) + \omega^{2}\Phi_{\rho} \Big] \end{aligned} \tag{A.9}$$

Appendix B

Partial derivatives calculation

Remark. The expressions f^{eom}_q, f^{eom}_v, and $f^{\text{eom}}_{\rho_i}$ denote the partial derivatives of f^{eom} with respect to the subscripted variables. The partial derivatives $\partial f^{\text{eom}}/\partial\zeta$ are obtained by differentiating f^{eom} with respect to $\zeta \in \{q, v, \rho\}$:

$$\frac{\partial f^{\text{eom}}}{\partial \zeta} = \frac{\partial(\mathsf{M}^{-1}\,\mathsf{F})}{\partial \zeta} = -\mathsf{M}^{-1}\mathsf{M}_\zeta\mathsf{M}^{-1}\,\mathsf{F} + \mathsf{M}^{-1}\,\mathsf{F}_\zeta = \mathsf{M}^{-1}\,\left(\mathsf{F}_\zeta - \mathsf{M}_\zeta\, f^{\text{eom}}\right) = \mathsf{M}^{-1}\,\left(\mathsf{F}_\zeta - \mathsf{M}_\zeta\,\dot{v}\right). \tag{B.1}$$

Remark. The expressions $\tilde{g}_q$, $\tilde{g}_v$, and $\tilde{g}_{\rho_i}$ denote the partial derivatives of $\tilde{g}$ with respect to the subscripted variables. The partial derivatives $\partial\tilde{g}/\partial\zeta$ are obtained by differentiating (3.1) with respect to $\zeta \in \{q, v, \rho\}$:

$$\begin{aligned}\tilde{g}_\zeta &= g_\zeta + g_{\dot{v}}\, f^{\text{eom}}_\zeta + g_{\tilde{u}}\, \tilde{u}_\zeta \\ &= g_\zeta + g_{\dot{v}}\, f^{\text{eom}}_\zeta + g_u\, u_\zeta\, + g_u\, u_{\dot{v}}\, f^{\text{eom}}_\zeta\end{aligned} \tag{B.2}$$

Which leads to

$$\begin{aligned}\left[\, \tilde{g}_q\; Q_i + \tilde{g}_v\; V_i + \tilde{g}_{\rho_i}\, \right]_{i=1,\ldots,p} \Leftrightarrow & \Big[\big(g_q + g_{\dot{v}}\, f^{\text{eom}}_q + g_u\, u_q\, + g_u\, u_{\dot{v}}\, f^{\text{eom}}_q\big) \cdot Q_i \\ & + \big(g_v + g_{\dot{v}}\, f^{\text{eom}}_v + g_u\, u_v\, + g_u\, u_{\dot{v}}\, f^{\text{eom}}_v\big) \cdot V_i \\ & + g_{\rho_i} + g_{\dot{v}} \cdot f^{\text{eom}}_{\rho_i} + g_u\, u_\rho\, + g_u\, u_{\dot{v}}\, f^{\text{eom}}_{\rho_i}\Big]_{i=1,\ldots,p}\end{aligned} \tag{B.3}$$

Remark. Similarly, the expressions $\tilde{w}_q$, $\tilde{w}_v$, and $\tilde{w}_{\rho_i}$ denote the partial derivatives of $\tilde{w}$ with respect to the subscripted variables. The partial derivatives $\partial\tilde{w}/\partial\zeta$ are obtained by differentiating w with respect to $\zeta \in \{q, v, \rho\}$:

$$\begin{aligned}\tilde{w}_\zeta &= w_\zeta + w_{\dot{v}}\, f^{\text{eom}}_\zeta + w_{\tilde{u}}\, \tilde{u}_\zeta \\ &= w_\zeta + w_{\dot{v}}\, f^{\text{eom}}_\zeta + w_u\, u_\zeta\, + w_u\, w_{\dot{v}}\, f^{\text{eom}}_\zeta\end{aligned} \tag{B.4}$$

Appendix C

Case study: Presentation of a five-bar mechanism

The five-bar mechanism with two degrees of freedom, shown in Fig. C.1a, is used as a case study to illustrate the sensitivity analysis approach for hybrid constrained multibody systems developed herein. The mechanism has five revolute joints located at points A, 1, 2, 3, and B where A and B are pinned. The fixed link between the two pinned points represent the fifth bar of the system. The state vector includes the natural coordinates of the point 1, 2, and 3 of the mechanism with $q = \left[q_1^{\mathrm{T}}\ q_2^{\mathrm{T}}\ q_3^{\mathrm{T}}\right]^{\mathrm{T}}$, where $q_2 = \left[x_2\ y_2\right]^{\mathrm{T}}$ represents the two degrees of freedom, and $q_1 = \left[x_1\ y_1\right]^{\mathrm{T}}$ with $q_3 = \left[x_3\ y_3\right]^{\mathrm{T}}$ represent the dependent coordinates. The dependent coordinates are solved using the constraints of the system. The constraints are defined according to the fixed lengths between each set of points, as follows:

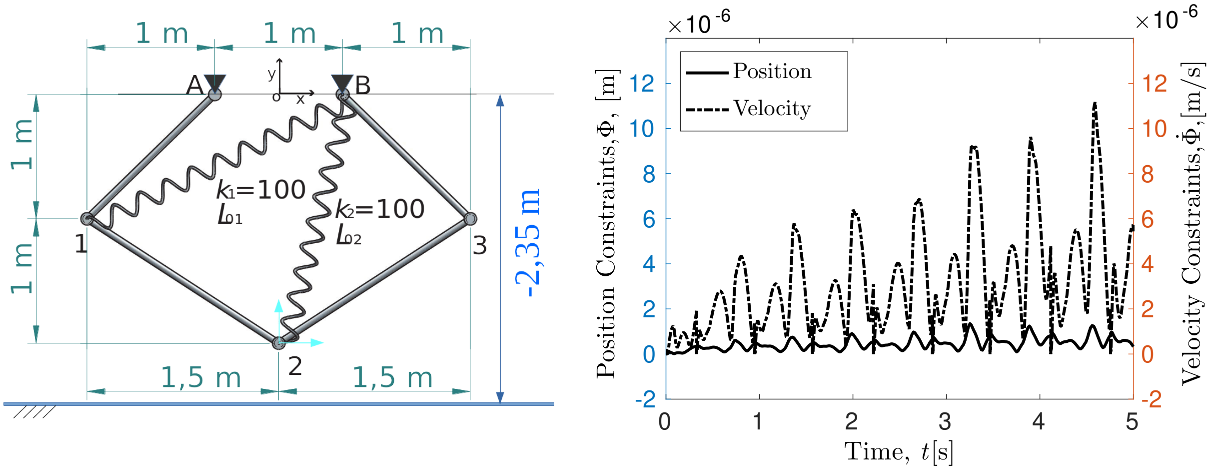
$$\Phi = \begin{bmatrix} \|q_A - q_1\|^2 - L_{A1}^2 \\ \|q_2 - q_1\|^2 - L_{21}^2 \\ \|q_3 - q_2\|^2 - L_{32}^2 \\ \|q_B - q_3\|^2 - L_{B3}^2 \end{bmatrix} = 0, \tag{C.1}$$

where the lengths $L_{A1} = L_{B3} = 1.4142\ m$; $L_{A1} = L_{B3} = 1.8027\ m$. The pinned points are located at $q_A = \begin{bmatrix} -0.5 & 0 \end{bmatrix}^{\mathrm{T}}$ and $q_B = \begin{bmatrix} 0.5 & 0 \end{bmatrix}^{\mathrm{T}}$. The masses of the bars are $m_1 = 1\ kg$, $m_2 = 1.5\ kg$, $m_3 = 1.5\ kg$, $m_4 = 1\ kg$; the polar moments of inertia are assumed to be ideal, with uniform distribution of mass; the two springs have stiffness coefficients of $k_1 = k_2 = 100\ N/m$ and natural lengths of $L_{01} = 2.2360\ m$ and $L_{02} = 2.0615\ m$.

A flat ground surface is located at -2.35 m and we define the event function $r\big(q|_{t_{\mathrm{eve}}}\big) = y_2 - y_{event} = 0$ (2.24), where the bottom point of the five-bar mechanism (point 2) hits the ground at $y_{event} = -2.35\ m$. Once the event is detected, the vertical velocity of point 2 jumps to its opposite value, while its horizontal velocity remains unchanged. This study computes the sensitivity of the bottom point of the five-bar mechanism (point 2) with respect to a small change in the initial lengths of the springs.

The canonical ODE for multibody systems (2.68) that computes the penalty ODE formulation for constrained multibody dynamics systems (2.66) and the sensitivities of such formulation is simulated for a time span of five seconds. The initial conditions for the two degrees of freedom were set randomly at $q_{2_{init}} = \left[\begin{array}{cc} 0.53029 & -2.10283 \end{array}\right]^{\mathrm{T}}$.

Figure C.1b shows the residuals of the constraint equations. The position constraints are satisfied within an error of 10^{-6}, while the velocity constraints are within and error of 10^{-5}, which is acceptable.

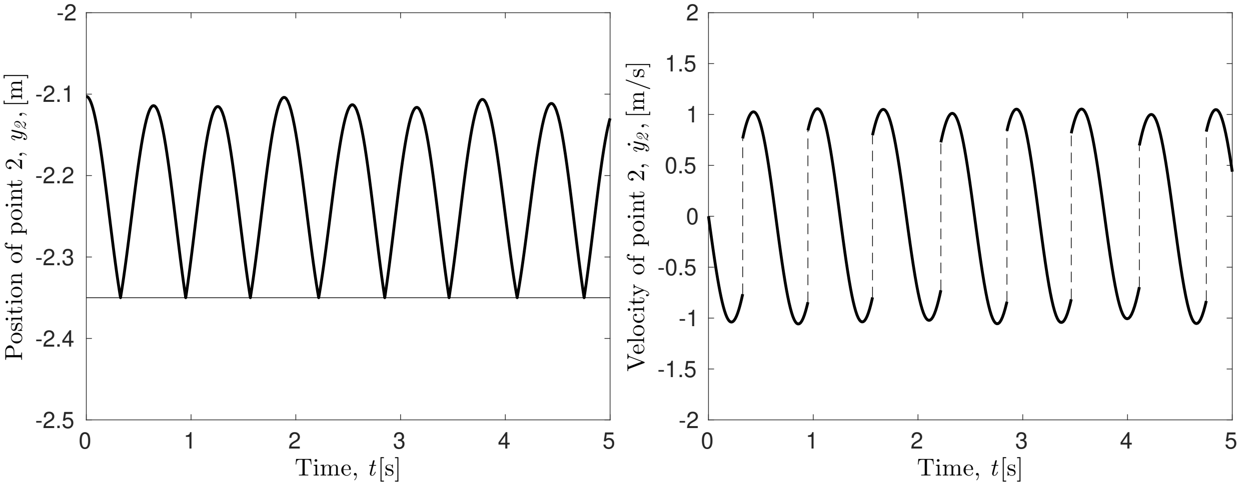


(a) Diagram of the five-bar mechanism

(b) The position and the velocity constraint residuals for the five-bar mechanism

Figure C.1: Structure of the five-bar mechanism

The trajectories of the position and velocity of point 2 of the five-bar mechanism along the vertical y axis are shown in Fig. C.2a and Fig. C.2b, respectively. These results show that point 2's vertical position bounces at -2.35m, as expected, and its vertical velocity jumps to its opposite value at each time of event.



(a) The vertical position of the bottom point y_2 of the five-bar mechanism

(b) The vertical velocity of the bottom point $\dot{y}_2$ of the five-bar mechanism

Figure C.2: Trajectories of the position and velocity of the bottom point the five-bar mechanism

Appendix D

Adjoint of the algebraic Lagrangian coefficient

Methods to compute the adjoint of an index-1 DAE available in the literature [65, 61, 66] use the following approach. Define the Lagrangian using the multipliers μ^Q, μ^V, μ^Γ that correspond to the constraints posed by the index-1 DAE equations (3.35):

$$\begin{bmatrix} \mu^Q \\ \mu^V \\ \mu^\Gamma \end{bmatrix}^T \cdot \left(\begin{bmatrix} \mathsf{I} & \mathsf{0} & \mathsf{0} \\ \mathsf{0} & \mathsf{M}\left(t, q, \rho\right) & \Phi_q^{\mathrm{T}}\left(t, q, \rho\right) \\ \mathsf{0} & \Phi_q\left(t, q, \rho\right) & \mathsf{0} \end{bmatrix} \cdot \begin{bmatrix} \dot{q} \\ \dot{v} \\ \mu \end{bmatrix} - \begin{bmatrix} v \\ \mathsf{F}\left(t, q, v, \rho\right) \\ \mathsf{C}\left(t, q, v, \rho\right) \end{bmatrix} \right) . \tag{D.1}$$

We rearrange equation (D.1) as follows:

$$\left(\begin{bmatrix}\mu^Q\\\mu^V\\\mu^\Gamma\end{bmatrix}\cdot\begin{bmatrix}\mathsf{I}&\mathsf{0}&\mathsf{0}\\\mathsf{0}&\mathsf{M}(t,q,\rho)&\Phi_q^{\mathrm{T}}(t,q,\rho)\\\mathsf{0}&\Phi_q(t,q,\rho)&\mathsf{0}\end{bmatrix}\right)\cdot\left(\begin{bmatrix}\dot{q}\\\dot{v}\\\mu\end{bmatrix}-\begin{bmatrix}\mathsf{I}&\mathsf{0}&\mathsf{0}\\\mathsf{0}&\mathsf{M}(t,q,\rho)&\Phi_q^{\mathrm{T}}(t,q,\rho)\\\mathsf{0}&\Phi_q(t,q,\rho)&\mathsf{0}\end{bmatrix}^{-1}\cdot\begin{bmatrix}v\\\mathsf{F}(t,q,v,\rho)\\\mathsf{C}(t,q,v,\rho)\end{bmatrix}\right) \tag{D.2}$$

$$=\left(\begin{bmatrix}\mu^Q\\\mu^V\\\mu^\Gamma\end{bmatrix}^T\cdot\begin{bmatrix}\mathsf{I}&\mathsf{0}&\mathsf{0}\\\mathsf{0}&\mathsf{M}(t,q,\rho)&\Phi_q^{\mathrm{T}}(t,q,\rho)\\\mathsf{0}&\Phi_q(t,q,\rho)&\mathsf{0}\end{bmatrix}\right)\cdot\left(\begin{bmatrix}\dot{q}\\\dot{v}\\\mu\end{bmatrix}-\begin{bmatrix}V\\f^{\text{DAE-}\dot{v}}\\f^{\text{DAE-}\mu}\end{bmatrix}\right) \tag{D.3}$$

$$=\begin{bmatrix}\lambda^Q\\\lambda^V\\\lambda^\Gamma\end{bmatrix}^T\cdot\left(\begin{bmatrix}\dot{q}\\\dot{v}\\\mu\end{bmatrix}-\begin{bmatrix}V\\f^{\text{DAE-}\dot{v}}\\f^{\text{DAE-}\mu}\end{bmatrix}\right). \tag{D.4}$$

The adjoint variables $\lambda^Q, \lambda^V, \lambda^\Gamma$ defined in this paper, and the adjoint variables μ^Q, μ^V, μ^Γ used in the literature (D.1), are related by the following matrix multiplication:

$$\begin{bmatrix}\lambda^Q\\\lambda^V\\\lambda^\Gamma\end{bmatrix}=\begin{bmatrix}\mathsf{I}&\mathsf{0}&\mathsf{0}\\\mathsf{0}&\mathsf{M}(t,q,\rho)&\Phi_q^{\mathrm{T}}(t,q,\rho)\\\mathsf{0}&\Phi_q(t,q,\rho)&\mathsf{0}\end{bmatrix}\cdot\begin{bmatrix}\mu^Q\\\mu^V\\\mu^\Gamma\end{bmatrix}.$$

The adjoint DAE equations and boundary conditions in the "μ formulation" [65, 61, 66] can be derived from the equations and boundary conditions in the "λ formulation" discussed in this paper, and vice-versa.

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