Structural optimization of flexible components within a multibody dynamics approach

Thesis submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Engineering Sciences

by

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Abstract

Structural optimization techniques rely on mathematical foundations in order to reach an optimized design in a rational manner. Nowadays, these techniques are commonly used for industrial applications with impressive results but are mostly limited to (quasi-)static or frequency domain loadings. The objective of this thesis is to extend structural optimization techniques to account for dynamic load cases encountered in multibody applications.

The thesis relies on a nonlinear finite element formalism for the multibody system simulation, which needs to be coupled with structural optimization techniques to perform the optimization of flexible components in an integrated way. To tackle this challenging optimization problem, two methods, namely the fully and the weakly coupled methods, are investigated.

The fully coupled method incorporates the time response coming directly from the MBS in the optimization. The formulation of the time-dependent constraints are carefully investigated as it turns out that it drastically affects the convergence of the optimization process. Also, since gradient-based algorithms are employed, a semi-analytical method for sensitivity analysis is proposed.

The weakly coupled method mimics the dynamic loading by a series of equivalent static loads (ESL) whereupon all the standard techniques of static response optimization can be employed. The ESL evaluation strongly depends on the formalism adopted to describe the MBS dynamics. In this thesis, the ESL evaluation is proposed for two nonlinear finite element formalisms: a classical formalism and a Lie group formalism.

An original combination of a level set description of the component geometry with a particular mapping is adopted to parameterize the optimization problem. The approach combines the advantages of both shape and topology optimizations, leading to a generalized shape optimization problem.

The adopted system-based optimization framework supersedes the classical component-based approach as the interactions between the component and the system can be consistently accounted for.
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Chapter 1

Introduction

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1.1 Context of the thesis

In the industry, engineers continuously face the challenge of providing high quality solutions that satisfy numerous requirements, often antagonistic. For instance, in many applications, the goal is to design the lightest component with the strongest mechanical resistance while achieving the lowest production cost. In the past, trial-and-error approach was commonly used to design a satisfactory solution. However, these methods are expensive, time consuming and there is no guarantee to reach an optimized design. Concurrently to the development of numerical tools, analysis capabilities have been improved whereupon automatic design methods were developed to obtain the best solution in a rational way and to remove the arbitrary component of trial-and-error methods from the design process. Nowadays, in high technology industries such as aerospace and automotive sectors, structural optimization techniques are commonly employed to design the best solution resulting from a trade-off between various design criteria.

Traditionally, the structural optimization of mechanical system components is performed using a component-based approach, i.e. the interactions between the optimized component and its environment (system) are often disregarded. For instance, to minimize the mass of a suspension upper-arm, the arm is first isolated from the vehicle and then a set of representative static loads with appropriate boundary conditions
are applied to the component, so that they mimic the complex loading to which it is subjected. Generally, these loads derive from the designer’s experience, from experiments or from standards. Dynamic amplification factors or safety factors are generally introduced to account for unmodeled phenomena. The resulting heuristic design criteria can be justified in incremental design procedures, wherein the experience from the past is relevant for the new design. However, it becomes clearly questionable when addressing innovative designs and breakthroughs. Also, albeit the component-based approach stands when the overall system can be considered as stiff, the approach is arguable when flexibility effects become larger. Indeed, with the design of lighter and more flexible components, the interactions between the system components play a more important role on the system dynamics and they can no longer be neglected. Therein, the component-based approach should be extended to account for the dynamic behavior of the entire system.

The analysis of mechanical systems accounts for the large relative displacement of their interconnected components. The earliest formulations were based on the assumptions that all the system components behave as rigid bodies. However, under high static forces and/or high speed motion, this assumption leads to discrepancies in the responses. Therein, the need of introducing flexibility within the analysis was rapidly motivated (Erdman et al., 1972). Later on, *multibody system dynamic formulations* have been developed to capture the compliant effects of the flexible bodies on the gross motion of the system in an integrated approach (Géradin and Cardona, 2001; Bauchau, 2011; Shabana, 2013).

This thesis is concerned with a *system-based approach* replacing and superseding the traditional component-based approach. This more advanced approach takes advantage of the evolution of virtual prototyping. It combines the capabilities of modern multibody system (MBS) simulation tools with structural optimization techniques to perform an integrated optimization of flexible components. Figure 1.1 illustrates the system-based approach.

The present work has been mainly realized in the framework of a research project, namely the LightCar project, that was launched in 2011 and sponsored by the pole of competitiveness “Mecatech” and the Walloon Region of Belgium. The aim of the project was to developed a virtual prototyping platform for the integrated analysis and optimization of vehicles. Industrial partners were interested to collaborate as well as to validate the contribution of the thesis. Industrial collaborations with Toyota Motor Corporation and Jtekt Torsen companies were specifically developed to optimize powertrain components.
1.2 Literature review

1.2.1 From mechanism synthesis to structural optimization

The design of a mechanism able to perform a desired task can be performed by mechanism synthesis techniques which define the mechanism at a system level in the conceptual design phase, i.e. the design variables are “global” such as the dimensions of the system, the number and the nature of kinematics joints, etc. The precise design of each component is addressed in a next step. The mechanism synthesis is generally performed using the static or kinematic response of the system considering rigid or flexible components. (see for instance, Erdman et al., 1972; Imam and Sandor, 1975; Cleghorn et al., 1981; Sohoni and Haug, 1982; Haug and Sohoni, 1984; Erdman and Sandor, 1991; Hansen, 1992; Hansen and Tortorelli, 1996; Sigmund, 1997; Hansen and Hansen, 1998; Minnaar et al., 2001; Hansen, 2002; Kawamoto, 2005; Sedlacek et al., 2005; Jensen and Hansen, 2006; Pucheta and Cardona, 2007; Cugnon et al., 2009; Collard et al., 2010; McCarthy and Soh, 2011). Some of these studies also incorporated structural parameters such as the areas of cross section in the optimization process to achieve mechanical requirements.

Once the mechanism is defined at a system level, two other more detailed design problems can be addressed. The first design problem concerns the optimal control of mechanisms, which aims at establishing the motor control laws, i.e. the actuator forces as a function of time, such that a certain optimality criterion is achieved (see for in-
stance, Okubo and Tortorelli, 2004; Albers et al., 2007; Held and Seifried, 2010; Seifried, 2012; Bastos Jr. et al., 2013). The second design problem is the structural optimization of components that modifies some structural parameters to satisfy design requirements. For instance, a typical problem is to minimize the mass of a component by varying several structural parameters subject to a limit on the maximum value of the stresses. This latter tool is the main concern of the thesis and is hereafter reviewed.

1.2.2 System-based approach for the structural optimization of MBS

Taking advantage of the evolution of MBS simulation tools, Bruns and Tortorelli (1995) initiated an approach combining rigid MBS analysis and optimization techniques to perform the structural optimization of components with load cases evaluated during the MBS analysis. The method was illustrated on the design of a slider-crank mechanism loaded with the maximum tensile force calculated during the simulation. Almost at the same period, Oral and Kemal Ider (1997) investigated the optimization problem that incorporates the dynamic response coming from the MBS analysis using a dynamic recursive formulation (Ider and Amirouche, 1989). They represented the time-dependent constraints either by the most critical constraint or agglomerated with a Kresselmeier-Steinhauser function. To perform the structural optimization of MBS, Etman et al. (1998) applied the approximation concepts instead of considering a direct coupling between the MBS analysis and the optimizer. They used linear approximations of the responses with respect to intermediate variables, and a combination of a constraint screening strategy with pointwise constraints to treat the time-dependent constraints. They validated the approach and illustrated it on several mechanisms.

Nowadays, the structural optimization of MBS can be divided into two main methods: the weakly coupled and the fully coupled. The weakly coupled method deals with a static response optimization wherein the dynamic response is mimicked by a set of equivalent static scenarios derived from the MBS simulation. On the other hand, the fully coupled method concerns the optimization problem which incorporates the time response coming directly from the MBS analysis.

Weakly coupled method

The beginnings of the weakly coupled method have been initiated by Saravanos and Lamancusa (1990) to perform the structural optimization of robotic arms. The authors selected several configurations of the mechanism whereupon the optimization was carried out based on representative static loading conditions coming from the designer’s experience for each posture. Even if the strategy tries to account for the entire system, this approach is non-rational since a few configurations can hardly represent the overall motion as well as the various operating conditions. Moreover, the optimal design entirely depends on the designer’s choices.

The transformation of the dynamic response into a set of equivalent static scenarios has been properly defined with the incorporation of the MBS analysis in the optimization
process. This transformation is realized in a two step approach. Firstly, a MBS simulation is performed whereby the loads applied to each component can be computed. Secondly, each component is optimized independently using a quasi-static approach in which a series of static load cases evaluated at the first step are applied to the respective components. The equivalent static loads are fixed during the optimization whereas they are design-dependent. Hence, cycles between the MBS analysis and the optimization are needed to account for this dependence. The weakly coupled method sounds appealing as it circumvents solving the complex dynamic response optimization problem. However, the method focuses on the optimization of isolated components wherein the load cases stem from the system analysis. A series of works were realized in which a couple of load cases associated to the reaction forces of the kinematic joints and boundary conditions were evaluated during the MBS analysis, and then considered for the static optimization process (Häussler et al., 2001, 2004; Albers et al., 2002). This approach has also been combined with lifetime prediction - durability analysis (Ilzhöfer et al., 2000; Albers and Häussler, 2005).

An important breakthrough has been made by Kang et al. (2005) who proposed a method to define Equivalent Static Loads (ESL) for the optimization of flexible mechanisms. For each time step and for each optimized component, they define an ESL producing the same displacement field as the one generated by the dynamic load at the considered time step in a body-attached frame. However, even if the concept seems totally general, it has been developed for MBS based on a floating frame of reference formulation. This formalism separates the elastic coordinates from the coordinates describing the global motion of the bodies which enables to define the ESL for each optimized component by simply isolating some terms of the equations of motion. The ESL approach has been employed in numerous studies with conclusive results (Kang et al., 2007; Witteveen et al., 2009; Hong et al., 2010; Sherif and Irschik, 2010) and is used in commercial software tools.

**Fully coupled method**

In lieu of solving an equivalent static optimization problem, the fully coupled method incorporates the time response coming directly from the MBS simulation. Therein, the optimization considers the system as a whole instead of isolated components as encountered with the weakly coupled method. The fully coupled method leads to dynamic response optimization problems which are more challenging to solve than classical structural optimization problems chiefly due to the difficulties of evaluating the dynamic response and then incorporating it in the optimization (Haug and Arora, 1979). Indeed, the treatment of time-dependent constraints is an essential issue as well as the computation of the sensitivities of the displacements, velocities and accelerations, that can become extremely costly (Park, 2007). Also, the local or global approximation of the original problem used in response surface methods or mathematical programming approaches is more complex as early reported by Etman (1997); Kurtaran and Eskandarian (2001); Marklund and Nilsson (2001); Kurtaran et al. (2002); Hong and
Chapter 1. Introduction

Park (2003). The fully coupled problem can be solved using either the conventional nested approach or the SAND (Simultaneous ANalysis and Design) approach (Haftka and Gürdal, 1992). In the conventional nested formulation, only the design variables are treated as optimization variables whereas the state variables are solved by forward integration. With the SAND formulation, the design variables and the state variables are treated as optimization variables. In the present research, the nested formulation is employed.

Regarding the structural optimization of structures considering transient loads, comprehensive studies were initiated in the seventies. Before the early seventies, the frequency response was predominant. Nowadays, dynamic response optimization is still a field of active research. One of the earliest work has been proposed by Fox and Kapoor (1970) who minimized the weight of frame structures subject to base motion and constraints on dynamic stresses and displacements. One must also cite the works of Willmert and Fox (1974), Afimiwala and Mayne (1974) and Feng et al. (1977) as well as the literature survey realized by Pierson (1972). Later on, Cassis and Schmit (1976) applied the concepts of approximation to incorporate the dynamic responses. Interested readers may refer to the review article written by Kang et al. (2006) for further details.

Focusing on the structural optimization of mechanical systems, Pereira and Dias (2003) employed the fully coupled method to solve optimization problems with crashworthiness and dynamic requirements. Later on, Brüls et al. (2011b) took advantage of the evolution of numerical simulations and topology optimization to design structural components within a flexible MBS simulation. They showed the feasibility and convenience of integrating the flexible MBS simulation directly in the optimization loop. Indeed, the dynamic effects are naturally incorporated into the design. Amongst other recent works, Seifried and Held (2011) used the fully coupled approach to optimize controlled flexible MBS. Durability-based constraints have also been considered in the fully coupled work of Tobias et al. (2010). They avoid post-processing the MBS simulation results by evaluating the damage values during the MBS simulation to hasten their computations. Other contributions about the fully coupled method have been realized with the PhD theses of Wang (2006) who investigated alternative formulations of the optimization problem and Dong (2012) who explored the topology optimization for multi-functional components in MBS.

1.3 Motivations, assumptions and objectives of the thesis

The present thesis continues along the study initiated by Brüls et al. (2011b) wherein the authors employed a fully coupled approach to design optimal components of MBS described using a classical nonlinear finite element formalism (Géradin and Cardona, 2001). The mechanism synthesis aspect is not considered by assuming that the mechanical system has a fixed configuration and topology (at the system level). Also, the
1.3 Motivations, assumptions and objectives of the thesis

optimal control is not directly treated in this thesis but future works are foreseen to couple structural optimization and optimal control.

The design of lighter and more flexible mechanical systems requires more advanced and more accurate numerical tools for the analysis but also for the design of optimal components. The use of a nonlinear finite element formalism provides a general framework to analyze complex mechanical systems wherein the flexibility is naturally taken into account. This contrasts with most of the previously cited studies wherein the MBS dynamics was described with a floating frame of reference formulation or rigid body MBS formulations.

The first two objectives of this thesis are related to the fully coupled approach for the optimization of MBS described using a classical nonlinear finite element formalism. As a dynamic response optimization is involved, the treatment of time-dependent constraints is a central issue to formulate properly the optimization problem. The first objective is to investigate the formulation of the optimization problem in order to conduct robust and effective optimization runs. Local formulations, enforcing constraints at each time step, and global formulations, agglomerating the responses into a few constraints, are studied. Secondly, the sensitivity analysis method is revisited. Indeed, the sensitivity analysis can drastically affect the computation time of the optimization process. Employing a basic finite difference scheme requires one additional simulation per design variable at each optimization iteration whereby the CPU grows by a factor $n_v + 1$, where $n_v$ numbers the design variables. This is especially pertinent with the fully coupled approach since the MBS simulation time is much larger than for a static analyses. Furthermore, for nonlinear systems, the derivative can be wrong if a bifurcation of the response occurs. Hence, a novel semi-analytical sensitivity analysis is proposed to compute the gradients in an efficient and simplistic manner.

A third objective concerns the parameterization of the design problem, which directly affects the performance of the optimization process. In this thesis, an implicit representation of the component geometry based on the level set method is proposed to design MBS components. The resulting optimization method can be qualified as a generalized shape optimization method as the component boundaries are smooth and topology changes are possible in a limited manner. While this description is totally general, our research has been conducted using the fully coupled approach. However, the proposed parameterization is independent of the optimization method and can thus be handily employed with other optimization methods.

The last set of objectives focuses on the weakly coupled approach. The ESL method was developed based on a floating frame of reference formulation (Kang et al., 2005). This formalism possesses inherent properties that enable to evaluate efficiently the ESL. Adapting the ESL evaluation to a classical nonlinear finite element formalism is not straightforward. The fourth objective is to propose a method to evaluate the ESL for MBS dynamics described using a classical nonlinear finite element formalism
(Géradin and Cardona, 2001). As an alternative, a nonlinear finite element approach based on a Lie group formalism (Sonneville and Brüls, 2014) is selected as it exhibits a number of attractive properties. Therein, the fifth objective is to take advantage of these properties to develop an efficient method to evaluate the ESL. The last objective is to conduct a fair comparison between the weakly and the fully coupled methods to point out the advantages and drawbacks of each method.

The main thread of the objectives targeted by the thesis is illustrated in Figure 1.2 which also depicts the flowchart of the thesis organization.

The MBS simulations are performed using the nonlinear finite element software Samcef Mecano\(^1\) or using MBS simulation tools developed at the University of Liège using Matlab (The MathWorks, Inc., 2012b). The optimization processes are conducted either using the optimization shell Boss Quattro\(^2\) or using scripts in Matlab (The MathWorks, Inc., 2012b).

### 1.4 Layout of the thesis

After this introductory chapter, Chapter 2 presents the fundamental tools used in this thesis, and is composed of two distinct sections. The first section presents the MBS analysis and gives an overview of the methods employed to formulate and solve the equations of motion. The second section introduces the basic principles of structural optimization and gives an insight into the main methods that are hereafter employed to perform the structural optimization of MBS components.

Chapter 3 summarizes the work carried out in this thesis. It introduces the MBS optimization wherein the different methods are detailed. The main results are briefly presented and glimpse the issues treated in the articles included as appendices. The main methods to perform the MBS component optimization are discussed based on the experience accumulated during the thesis.

Chapter 4 briefly summarizes the work that is performed in each of the four articles and the original contributions and impact of the present thesis are detailed. Finally, Chapter 5 concludes the thesis and points out several directions for future work.

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1.4 Layout of the thesis

Figure 1.2: Flowchart of the thesis organization.

- MBS structural optimization
- Fully coupled approach
  - Dynamic response optimization
- Weakly coupled approach
  - Static response optimization using the ESL method
- Nested approach
- SAND approach
- Component level optimization
  - ESL approach
  - Lie group formalism
- System level optimization
  - ESL approach
  - Incorporating function
- Treatment of time-dependent functions
- Level set description
- Level set description
- Level set description
- Sensitivity analysis
- Optimal Control
- Perspective

Article 1

Article 2

Article 3

Article 4
Chapter 2

Fundamental Tools

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This research is developed in a computer-aided engineering (CAE) framework involving notably computer-aided design, multibody system dynamics, structural optimization and sensitivity analysis. This chapter introduces the fundamental tools that are later on coupled to perform the integrated optimization of flexible components within a MBS approach.

First, the flexible multibody system analysis is presented. The choice of the reference frame is discussed and the equations of motion as well as the time integration scheme are described. Afterwards, structural optimization is introduced wherein the design parameterization, the problem formulation and the solution algorithms including the sensitivity analysis are discussed.
2.1 Multibody system analysis

2.1.1 Introduction to MBS simulation

A flexible multibody system (MBS) can be defined as a collection of rigid and flexible bodies interconnected by rigid and flexible kinematic joints (e.g. revolute, prismatic or universal joints) and by force elements (e.g. springs or dampers). A basic multibody system is depicted in Figure 2.1. The analysis of such systems may involve strong couplings between the gross motion and deformations within the system.

Figure 2.1: Multibody system diagram.

Owing to the research carried out the last decades and the growth of computational resources, mechanisms are nowadays commonly analyzed using multibody system simulation tools. Forward dynamics of MBS is the most usual approach and consists in understanding how the systems move under the influence of forces. Conversely, the inverse dynamics studies the forces that are needed to move the system in a desired manner.

Numerous fields of engineering call for MBS analyses. Classical applications are encountered in robotics, e.g. to simulate the robot trajectory (Dwivedy and Eberhard, 2006), in aerospace, e.g. to analyze the deployment of antennas (Li, 2012) or in machining process to predict the manufacturing performance (Zaeh and Siedl, 2007). In air and ground transport sectors, MBS analyses are also extensively employed with applications in aeronautics (Doan, 2004; Bottasso et al., 2006; Krüger and Morandini, 2011) in automotive (Virlez, 2014; Blundell and Harty, 2015) and in railways (Docquier et al., 2007). More recently, the development of sustainable energy systems motivates accurate multibody models of wind turbines (Heege et al., 2007; Helsen et al., 2014; Schulze et al., 2014). Finally, biomechanics recently pushes forward the development of MBS simulation methods wherein researchers simulate the dynamics of human body (Grosu et al., 2014; Quental et al., 2015).
Independently of the underlying approach adopted to analyze the MBS dynamics, the simulation process is composed of 4 steps:

1. Modeling assumptions and definition of the boundary conditions,
2. Element formulation and generation of the equations of motion,
3. Time-integration of the system of equations,
4. Interpretation of the results.

The first step involves the engineer’s capabilities to determine the components that should be incorporated in the MBS model in order to perform an accurate and efficient dynamic analysis, matching his desiderata. The analysis of a crankshaft is illustrated in Figure 2.2. Only a limited number of engine parts are necessary to simulate the dynamic behavior of the crankshaft considering a desired level of accuracy. Furthermore, the designer makes assumptions on the behavior of each component, e.g. the piston flexibility can be neglected and it is assumed to behave as a rigid body. Within this step, the designer also determines the boundary conditions to perform the simulation and the material properties of each component.

The second step mainly concerns the element formulation wherein the kinematics of each element (body, joint, etc) is described using a set of coordinates. All the forces
Chapter 2. Fundamental Tools

generated inside the element must be expressed as functions of the coordinates and their time derivatives. In case of external forces or elements such as actuators, forces may explicitly depend on time. Several types of coordinates exist in the literature: minimal coordinates (Hiller and Kecskeméthy, 1994), relative coordinates (Samin and Fisette, 2003), reference point coordinates (Shabana, 2013), natural coordinates (de Jalón, 2007) and finite element coordinates (Géradin and Cardona, 2001). The choice of a coordinate set is fundamental as it determines the form and the dimension of the equations describing the physical system. Thusly, the computational efficiency and the implementation ease are directly related to this choice. Nevertheless, each set has its own advantages and drawbacks and the best choice depends on the application. In this research, the finite element coordinates, particularly well-suited for the description of flexibility, are used.

The third step chiefly implies computational resources. The equations of motion are assembled and the time-integration is performed.

The last step is dedicated to the analysis and the interpretation of the results. MBS simulations provide a lot of information, e.g. stresses, strains, reaction forces in kinematic joints, trajectory tracking, etc, which are accumulated during the simulation and can be post-processed. The engineer role is fundamental to take advantage of the MBS simulation results. First, the consistency and the accuracy of the mechanical responses must be checked whereupon the results can be interpreted and the conclusions drawn. Numerical results may be validated with experimental results or analytical models.

2.1.2 Several types of reference frames

Flexible MBS analysis aims at computing the elastic deflections of structural components undergoing large displacements, including large rotations, wherein the global motions and deformations are strongly coupled. The strain field is generally determined by means of shape functions (vibration modes or finite element shape functions) associated to a finite set of coordinates (amplitude of modes, position of nodes) arising from the spatial discretization of the flexible body. Depending on the reference frame wherein deformations are evaluated, several methods have been proposed in the literature to analyze both the large motions and the deformations in an integrated way, see Wasfy and Noor (2003) for a detailed review. Hereafter, the inertial frame, the floating frame and the corotational frame approaches are briefly introduced. The different approaches for an isolated component are depicted in Figure 2.3, which follows the classification proposed by Wasfy and Noor (2003).

The floating frame of reference method (Fig. 2.3(a)) may be interpreted as an extension of the analysis of rigid MBS in order to simulate flexible MBS (Shabana and Wehage, 1983). The motion of a flexible body is separated into a global rigid body motion represented by the floating frame of reference, and elastic deformations defined with respect to this body-attached frame (De Veubeke, 1976; Nikravesh and Lin, 2005;
2.1 Multibody system analysis

(a) Floating frame of reference.  
(b) Corotational frame.  
(c) Inertial frame.

<table>
<thead>
<tr>
<th>Rigid motions + deformations</th>
<th>No distinction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rigid + Elast. Coord.</td>
<td>Absolute Nodal Coordinates (FE)</td>
</tr>
</tbody>
</table>

Figure 2.3: Several types of reference frames.

Shabana, 2013). In case of small deformations, a linear elastic model can be used within the floating frame leading to compact and simple expressions of elastic forces. Model order reduction techniques may improve the simulation process by reducing the system size. Nonetheless, this formalism leads to a highly nonlinear inertia matrix because rigid and elastic coordinates are coupled by nonlinear terms. In case of more general situations, when the assumptions of small deformations and small velocities are no longer valid, the formalism suffers from a lack of accuracy and higher-order terms must be included to capture the geometrically nonlinear behavior of the system (Wallrapp and Schwertassek, 1991).

Following Shabana (2013), the equations of motion that govern a flexible MBS using a floating frame of reference formulation are expressed as

\[
\begin{bmatrix}
    m_{xx}^b & m_{x\theta}^b & m_{xf}^b \\
    m_{x\theta}^b & m_{\theta\theta}^b & m_{\theta f}^b \\
    m_{xf}^b & m_{\theta f}^b & m_{ff}^b
\end{bmatrix}
\begin{bmatrix}
    \ddot{x}_0^b \\
    \ddot{\theta}_0^b \\
    \ddot{q}_f^b
\end{bmatrix}
+ \begin{bmatrix}
    0 & 0 & 0 \\
    0 & 0 & 0 \\
    0 & 0 & K_{ff}^b
\end{bmatrix}
\begin{bmatrix}
    x_0^b \\
    \theta_0^b \\
    q_f^b
\end{bmatrix}
= 
- \begin{bmatrix}
    C_{x}^{T} \\
    C_{\theta}^{T} \\
    C_{q_f}^{T}
\end{bmatrix}
\lambda 
+ \begin{bmatrix}
    \left( g_{ext}^b \right)_x^{x} \\
    \left( g_{ext}^b \right)_\theta^{\theta} \\
    \left( g_{ext}^b \right)_f^{f}
\end{bmatrix}
+ \begin{bmatrix}
    \left( g_{vel}^b \right)_x^{x} \\
    \left( g_{vel}^b \right)_\theta^{\theta} \\
    \left( g_{vel}^b \right)_f^{f}
\end{bmatrix},
\]

\[b = 1, \ldots, n_b,\]

(2.1)

where \( n_b \) is the number of bodies, \( q_f \) is the set of flexible coordinates accounting for the deformations in the body-attached frame, \( x_0^b \) is a set of Cartesian coordinates that defines the origin location of the floating frame of reference and \( \theta_0^b \) is a set of rotational coordinates that describes the orientation of the floating frame of reference. The right-hand-side terms of Equation (2.1) are the reaction force vector \( C \) resulting from the
joint constraints, the external load vector $\mathbf{g}_{\text{ext}}$ and the quadratic velocity vector $\mathbf{g}_{\text{vel}}$ accounting for the effect of Coriolis and centrifugal forces.

In Equation (2.1), the separation between the two sets of coordinates is clearly highlighted. The first two rows concern the rigid body motion of body $b$ whereas the last row pertains to the flexibility of this body. This characteristic is the cornerstone of the Equivalent Static Load (ESL) method initially developed by Kang et al. (2005) to perform the structural optimization of flexible component in MBS. This is detailed in Articles [3]-[4] given in appendix.

Examples of MBS software tools based on this formalism are RecurDyn\textsuperscript{1}, Simpack\textsuperscript{2} or Robotran\textsuperscript{3}. These simulation tools were initially developed to perform rigid MBS simulation and were afterwards improved to account for component flexibility.

An inertial frame approach is typically adopted for classical nonlinear finite element formulations (Gérardin and Cardona, 2001; Bauchau, 2011), wherein absolute nodal coordinates are defined. These coordinates correspond to the displacements and orientations of each node of the finite element mesh (Fig. 2.3(c)). In contrast to the floating frame of reference approach, the resulting motion of the flexible MBS does not exhibit any decoupling between the global rigid body motion and the deformations. However, due to the geometric nonlinearities involved by large amplitude motions and deformations, this formulation requires a nonlinear elastic model even if the deformations are small in order to accommodate the nonlinear relation between the strains and the generalized coordinates. Nonetheless, the inertial frame approach eases the inertia force computation. This formulation is further developed in Section 2.1.3, as a classical nonlinear finite element formalism is mainly adopted in this thesis.

The corotational frame approach can be interpreted as a mixture between the inertial frame and the floating frame of reference approaches (Fig. 2.3(b)). It has been proposed to facilitate the computation of elastic forces in a nonlinear finite element model (Belytschko and Hsieh, 1973; Cardona and Geradin, 1991; Crisfield et al., 1997). Although the absolute nodal coordinates are used to determine the spatial configuration of the flexible body, a corotational frame is attached to each element of the finite element mesh and follows its gross motion. This approach is interesting as it combines the advantages of the two previous methods. First, despite the large displacements of flexible bodies, a linear elasticity model can be used at the element level in case of small deformations. Ergo, the computation of elastic forces is facilitated. Then, the generalized coordinates are not explicitly separated into a set defining the position of the body-attached frame and a set of flexible coordinates. The position and orientation of the corotational frame are determined as a function of the absolute nodal coordinates of the finite element nodes, which can be considered as intermediate variables describing

\textsuperscript{1}www.functionbay.org
\textsuperscript{2}www.simpack.com
\textsuperscript{3}wwwrobotran.be
the gross motion of the flexible body. A corotational description is also employed to formulate superelements within the nonlinear finite element method. The corotational frame approach is used in Article [3] in order to derive the equivalent static loads for MBS described using a classical nonlinear finite element formalism.

MBS simulation tools resulting from the last two approaches generally stem from the finite element community, and are available in the software Samcef Mecano\(^4\) for instance.

### 2.1.3 Classical nonlinear finite element approach for MBS dynamics

The standard nonlinear finite element formulation (Bauchau, 2011; Géradin and Cardona, 2001) is mainly adopted in this thesis to describe flexible MBS dynamics. The next two sections present the basic principles of the method.

This formulation stems from the finite element community that initially developed a robust theory for the analysis of a lone flexible component. Later on, the theory was generalized to analyze the dynamics of flexible MBS. As a result, the theory accounts for the flexibility and the nonlinear effects in a natural way. Also, the principles of the finite element method are recovered, i.e. the contributions to the equations of motion of each component and each kinematic joint are first expressed independently and are afterwards assembled via a systematic procedure. In the nonlinear finite element formalism, flexible components, rigid bodies as well as superelements can be mixed to obtain the best compromise between accuracy and computational efficiency.

#### Equations of motion

The equations of motion of flexible MBS are established from the Hamilton principle of mechanics. Let us assume that the potential energy of external forces \( V(q) \), the strain energy of elastic bodies \( W(q) \) and the kinetic energy defined by

\[
K(q, \dot{q}) = \frac{1}{2} \dot{q}^T M(q) \dot{q}
\]

of a flexible MBS are known. The vector \( q \) contains the displacements and orientations of each node of the finite element mesh, i.e. the absolute nodal coordinates in the inertial frame. We note that the symmetric mass matrix \( M \) may depend on the generalized coordinates due to the parameterization of the rotation variables. The Lagrangian function of the conservative system is defined as

\[
L(q, \dot{q}) = K(q, \dot{q}) - V(q) - W(q).
\]

By combining the Hamilton principle with the Lagrange function (2.3), the equations of motion can be derived. Hamilton principle states that the actual trajectory of the

unconstrained system between two time instants \( t_i \) and \( t_f \) is such that the variation of the integral is stationary provided that the initial and final configurations are fixed. However, since \( m \) kinematic constraints are enforced between generalized coordinates of the system, the trajectory is then a solution of the following constrained minimization problem

\[
\begin{align*}
\text{minimize} & \quad A = \int_{t_i}^{t_f} \mathcal{L} \, dt \\
\text{subject to} & \quad \Phi(q) = 0.
\end{align*}
\]

The term \( \Phi(q) \) is a set of algebraic equations imposing holonomic constraints between nodal coordinates, which typically represents the connections between bodies due to hinges, spherical joints, etc. The treatment of the more general case of non-holonomic constraints \( \Phi(q, \dot{q}, t) \) is described in e.g. Géradin and Cardona (2001).

Several methods exist to solve this type of problem. A possibility is to use the Lagrange multiplier method wherein additional unknowns, the Lagrange multipliers \( \lambda \), are associated to the algebraic equations \( \Phi \), transforming the constrained minimization problem into an unconstrained problem. Expressing the stationarity condition on this unconstrained problem leads to

\[
\delta \int_{t_i}^{t_f} \left( \mathcal{L} - \lambda^T \Phi \right) \, dt = 0.
\]

Integrating by part Equation (2.5) and remembering that the motion is specified at instants \( t_i \) and \( t_f \) yields

\[
\left( \frac{d}{dt} \left( \frac{\partial \mathcal{L}}{\partial \dot{q}} \right) - \frac{\partial \mathcal{L}}{\partial q} + C \right) \delta q + \delta \lambda^T \Phi = 0,
\]

where \( C \) represents the internal forces applied onto the generalized coordinates due to the holonomic constraints. These reaction forces \( C_i \) are expressed as

\[
C_i = \frac{\partial \Phi^T}{\partial q_i} \lambda.
\]

An augmented Lagrangian method can be employed to improve the numerical conditioning of the solution. The expression of \( C_i \) is modified by means of two terms, a scaling factor \( k \) and a penalty term \( p \Phi^T q \Phi \), leading to

\[
C_i = \Phi^T q (k \lambda + p \Phi T)
\]

where the subscript \((\bullet)_q\) denotes the derivative with respect to \( q \). The multiplication of the constraint equations by a scaling factor \( k \) creates matrices with terms of the same order of magnitude which avoids the ill-conditioning of the iteration matrix (Géradin and Cardona, 2001). The penalty term \( p \Phi^T q \Phi \) eases the convergence of the Newton-Raphson iterative process when \( \Phi \to 0 \). Since this term vanishes at convergence, the response of the system is independent of the choice of the penalty factor \( p \).
Introducing Equation (2.3) into Equation (2.6) and considering an augmented Lagrangian approach, the equations of motion finally take the general form of an index-3 differential-algebraic system (DAE)

\[ \begin{align*}
M(q) \ddot{q} + g^{gr}(q, \dot{q}) + g^{int}(q) + \Phi_q^T(q)(k\lambda + p\Phi(q)) &= g^{ext}(q), \\
k\Phi(q) &= 0,
\end{align*} \]

(2.9) \hspace{1cm} (2.10)

where \( q, \dot{q} \) and \( \ddot{q} \) are respectively the generalized displacement, velocity and acceleration vectors, and \( g^{ext}, g^{int} \) and \( g^{gr} \) are respectively the external, internal and complementary inertia forces. The set of Lagrange multipliers \( \lambda \) can be interpreted as the reaction forces needed to impose the algebraic constraints \( \Phi(q) = 0 \).

The equations of motion consist of a set of \( n \) nonlinear differential equations (2.9) supplemented by \( m \) algebraic equations (2.10) related to the kinematic and rigidity constraints. Nonlinearities arise from various origins: nonlinear material behavior, geometry, contact phenomena, etc. Thusly, at each simulation time step, the nonlinear DAE-system of \( n + m \) equations with \( n + m \) unknowns must be solved. The set of equations is often large since numerous generalized coordinates are involved but the global system matrices are sparse.

**Time integration scheme**

Numerical methods are employed to solve the equations of motion. Three families of time integration methods can be identified in the literature: the algorithms for first-order ODEs (multistep and Runge-Kutta methods), the algorithms for second-order ODEs (methods of the Newmark family) and structure-preserving methods (energy-preserving schemes and variational integrators). This section focused on an algorithm of the Newmark family, namely the generalized-\( \alpha \) method initially developed by Chung and Hulbert (1993), which is used in this research.

The Newmark family of methods has several advantages to solve stiff differential-algebraic equations as encountered with the analysis of flexible MBS due to kinematic constraints. Géradin and Cardona (2001) suggested to use the generalized-\( \alpha \) time integration scheme to solve the set of nonlinear DAE equations (2.9)-(2.10). Indeed, this method combines the advantages of one-step implementation, unconditional stability for linear problems, second-order accuracy and adjustable high-frequency numerical damping. Numerical damping is especially valuable to eliminate spurious high-frequency effects caused by the higher-order modes of a finite element model. Arnold and Brüls (2007) achieved a full convergence analysis in the DAE case and demonstrated that, despite the presence of algebraic constraints and the non-constant character of the mass matrix, the generalized-\( \alpha \) method leads to accurate and reliable results with a small amount of numerical damping.

The generalized-\( \alpha \) method is an implicit time integrator, i.e. at each time step, the computation of the generalized coordinates and their velocity requires the knowledge
of accelerations at the current time step. To ensure the stability of the numerical solution, implicit time integrators are preferable. Indeed, the crucial choice of the time step size is mainly governed by accuracy considerations as the high frequencies are filtered out by numerical damping.

At each time step of the MBS analysis, the numerical variables $q_{n+1}, \dot{q}_{n+1}, \ddot{q}_{n+1}$ and $\lambda_{n+1}$ must satisfy the residual equation

$$\begin{cases}
\text{res} \equiv M\ddot{q} + g + \Phi_q^T (k\lambda + p\Phi) = 0, \\
k\Phi = 0.
\end{cases} \quad (2.11)$$

In order to have the same number of equations as the number of unknowns ($q, \dot{q}, \ddot{q}, \lambda$), the equations of motion are supplemented by the Newmark integration formulae resulting from a Taylor series expansion of the displacement and velocity fields. According to the generalized-$\alpha$ method, a vector $a$ of acceleration-like variables is defined by the recurrence relation

$$\begin{align*}
(1 - \alpha_m) a_{n+1} + \alpha_m a_n &= (1 - \alpha_f) \ddot{q}_{n+1} + \alpha_f \ddot{q}_n, \\
(1 - \alpha_m) \dot{a}_{n+1} + \alpha_m \dot{a}_n &= (1 - \alpha_f) \dot{q}_{n+1} + \alpha_f \dot{q}_n.
\end{align*} \quad (2.12)$$

with $a_0 = \ddot{q}_0$. The vector $a_n$ is an auxiliary variable used by the algorithm and can be interpreted as an approximation of the true acceleration $\ddot{q}(t)$ at time $t = t_n + h (\alpha_m - \alpha_f)$ where $h$ denotes the time step. The time integration scheme is subsequently obtained by employing $a$ in the Newmark integration formulae

$$\begin{align*}
q_{n+1} &= q_n + h\dot{q}_n + h^2\left(\frac{1}{2} - \beta\right) a_n + h^2 \beta a_{n+1}, \\
\dot{q}_{n+1} &= \dot{q}_n + h (1 - \gamma) a_n + h \gamma a_{n+1}.
\end{align*} \quad (2.13)$$

If the parameters $\alpha_f, \alpha_m, \beta$ and $\gamma$ are properly chosen according to Chung and Hulbert (1993), second-order accuracy and unconditional stability are guaranteed for linear problems. It is convenient to define these parameters in terms of the spectral radius at infinite frequencies $\rho_\infty \in [0, 1]$ as

$$\begin{align*}
\alpha_m &= \frac{2\rho_\infty - 1}{\rho_\infty + 1}, \\
\alpha_f &= \frac{\rho_\infty}{\rho_\infty + 1}, \\
\gamma &= \frac{1}{2} - \alpha_m + \alpha_f, \\
\beta &= \frac{1}{4} \left(\gamma + \frac{1}{2}\right)^2.
\end{align*} \quad (2.15)$$

The choice $\rho_\infty = 0$ annihilates the high frequency response whereas $\rho_\infty = 1$ corresponds to no numerical damping.

To solve the implicit system of equation (2.11) at time $t_{n+1}$, a Newton-Raphson procedure is employed. Using a predictor-corrector scheme, the unknown response $(\ddot{q}, \dot{q}, q, \lambda)$ is divided into an approximate solution $(\ddot{q}^*, \dot{q}^*, q^*, \lambda^*)$ and a correction $(\Delta q, \Delta \dot{q}, \Delta q, \Delta \lambda)$
leading to

\[ q \rightarrow q^* + \Delta q, \]  
\[ \dot{q} \rightarrow \dot{q}^* + \Delta \dot{q}, \]  
\[ \ddot{q} \rightarrow \ddot{q}^* + \Delta \ddot{q}, \]  
\[ \lambda \rightarrow \lambda^* + \Delta \lambda. \]

where the subscript \( n+1 \) is dropped. The correction is computed based on the linearized form of the residual equation (2.11) around the approximate solution \((q^*, \dot{q}^*, \ddot{q}^*, \lambda^*)\) as

\[
\begin{bmatrix}
\text{res}^{\text{lin}}(q^* + \Delta q, \dot{q}^* + \Delta \dot{q}, \ddot{q}^* + \Delta \ddot{q}, \lambda^* + \Delta \lambda, t)
\end{bmatrix}
\begin{bmatrix}
\text{res}^*(q^*, \dot{q}^*, \ddot{q}^*, \lambda^*, t)
\end{bmatrix}
\begin{bmatrix}
M & 0 \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
\Delta \dot{q} \\
\Delta \lambda
\end{bmatrix}
\begin{bmatrix}
C_t & 0 \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
\Delta q \\
\Delta \lambda
\end{bmatrix}
\begin{bmatrix}
K_t & k \Phi_q^T \\
k \Phi_q & 0
\end{bmatrix}
\begin{bmatrix}
\Delta q \\
\Delta \lambda
\end{bmatrix} = 0,
\]

where \( C_t = \partial \text{res} / \partial \dot{q} \) and \( K_t = \partial \text{res} / \partial q \) denote respectively the tangent damping and stiffness matrices.

To solve Equation (2.20), the integration formulae (2.12)-(2.14) are manipulated by solving Equation (2.12) for \( a_{n+1} \) and inserting that result into Equations (2.13)-(2.14). The resulting two equations are

\[
\Delta \dot{q} = \frac{\gamma}{\beta h} \Delta q,
\]
\[
\Delta \ddot{q} = \frac{1}{\beta h^2} \left( 1 - \alpha_m \right) \Delta q.
\]

Using Equations (2.21)-(2.22), the linearized form of the update equation (2.20) reduces to

\[
S_t \begin{bmatrix}
\Delta q \\
\Delta \lambda
\end{bmatrix} = - \begin{bmatrix}
\text{res}^* \\
k \Phi^*
\end{bmatrix},
\]

where \( S_t \) is the tangent iteration matrix defined as

\[
S_t = \begin{bmatrix}
\frac{1 - \alpha_m}{1 - \alpha_f} \frac{1}{\beta h^2} M + \frac{\gamma}{\beta h} C_t + K_t & k \Phi_q^T \\
k \Phi_q & 0
\end{bmatrix}.
\]

Equation (2.23) is solved for the correction \((\Delta q, \Delta \lambda)\) and the approximate solution is updated, cf. Equations (2.16)-(2.19) and (2.21)-(2.22). Iterations continue until the residuals of Equation (2.11), \( \text{res} \) and \( \Phi \), are close to zero, i.e. until \( \| \text{res} \| < \text{tol}_{\text{res}} \) and \( \| \Phi \| < \text{tol}_{\Phi}. \)
Algorithm 1 summarizes the previous developments. We note that the process is initialized with $\lambda_{n+1} = 0$ and $\dot{q}_{n+1} = 0$. Initialization with the previous time step, i.e. $\dot{q}_{n+1} = \dot{q}_n$ and $\lambda_{n+1} = \lambda_n$, is also possible but does not significantly improve the convergence speed. The condition $it < it_{max}$ limits the number of iterations inside the iterative process.

**Algorithm 1 Generalized-\(\alpha\) time integration scheme**

1. Initialize values $q_0, \dot{q}_0$
2. Assign $\ddot{q}_0 = a_0 = 0$
3. for $n = 0$ to $n_{end}$ do
   - Assign $\dot{q}_{n+1} = 0, \lambda_{n+1} = 0$
   - Compute $a_{n+1}, q_{n+1}, \ddot{q}_{n+1}$ via (2.12)-(2.14)
   - while ($\|\text{res}\| < \text{tol}_r$ and $\|\Phi\| < \text{tol}_\Phi$ and $it < it_{max}$) do
     - Compute the residuals $\text{res}$ and $\Phi$
     - Compute the corrections via (2.23)
     - $\begin{bmatrix} \Delta q \\ \Delta \lambda \end{bmatrix} = -S_t^{-1} \begin{bmatrix} \text{res} \\ k\Phi \end{bmatrix}$
   - Increment $q, \dot{q}, \ddot{q}, \lambda$ via (2.16)-(2.19) and (2.21)-(2.22)
4. end while
5. $a_{n+1} = a_{n+1} + \frac{1 - \alpha_f}{1 - \alpha_m} \ddot{q}_{n+1}$, cf. (2.12)
6. end for

2.1.4 Lie group formalism for MBS dynamics

In a classical nonlinear finite element approach (Géradin and Cardona, 2001; Bauchau, 2011), the treatment of rotations is an important issue since large rotation motions are considered, leading to a non-trivial problem. To illustrate the complexity of the problem, one can observe the non-commutative property of the rotation matrix product, i.e. reversing the order of two successive rotations around two different axes leads to different geometric configurations of the object to which they are applied. Also, a parameterization of the rotation variables is needed and may strongly affect the efficiency of nonlinear computations as it depends on the adequacy of the set of parameters adopted (Bauchau and Trainelli, 2003). Moreover, singularities of the parameterization exist and require a careful consideration. In this section, a particular Lie group formalism is presented which, among others, circumvents the problem of rotation parameterization.

**Free rigid body motion analysis**

Before introducing the mathematical description of flexible MBS using a Lie group formalism, let us analyze the free 3D motion of a single rigid body as depicted in Figure 2.4. We assume the existence of a fixed inertial frame $\{O, X, Y, Z\}$. The motion of the rigid body can be described as the motion of a body-attached frame $\{O_A, x, y, z\}$
with respect to the inertial frame. According to the notation of Figure 2.4, geometric vectors are introduced to describe the position of an arbitrary point \( P \) of the rigid body, leading to

\[
\vec{x} = \vec{x}_{OA} + \vec{x}'.
\] (2.25)

![Figure 2.4: Free 3D motion of a single rigid body represented at three different configurations.](image)

The geometric vector \( \vec{x}' \) can be expressed either in the inertial frame by the \( 3 \times 1 \) algebraic vector \( \vec{x}' \) or in the body-attached frame by the \( 3 \times 1 \) algebraic vector \( \vec{X} \). These vectors satisfy

\[
\vec{x}' = \vec{R}\vec{X}
\] (2.26)

where \( \vec{R} \) is a \( 3 \times 3 \) rotation matrix. As a consequence, Equation (2.25) can be rewritten as

\[
\vec{x} = \vec{x}_{OA} + \vec{R}\vec{X}
\] (2.27)

which is the fundamental equation describing the rigid body kinematics. The rigid body transformation from a reference configuration to a configuration \( A \) is thus represented by a rotation matrix \( \vec{R} \) and a position vector \( \vec{x}_{OA} \). The transformation is defined via 6 parameters: 3 parameters are related to \( \vec{x}_{OA} \) and 3 parameters are related to \( \vec{R} \) where the orthogonality conditions have been considered, enforcing 6 independent constraints over the 9 initial parameters.

Using the homogeneous representation of vectors, the rigid body motion can be described in a compact way as

\[
\begin{bmatrix}
\vec{x} \\
1
\end{bmatrix} = \mathcal{H}(\vec{R}, \vec{x})
\begin{bmatrix}
\vec{X} \\
1
\end{bmatrix}
\] (2.28)
where the $4 \times 4$ matrix $\mathcal{H}(\mathbf{R}, \mathbf{x})$ is defined as

$$
\mathbf{H} = \mathcal{H}(\mathbf{R}, \mathbf{x}) = \begin{bmatrix} \mathbf{R} & \mathbf{x} \\ 0 & 1 \end{bmatrix}.
$$

(2.29)

It is worth noticing that the matrix $\mathbf{H}$ represents a frame transformation. Moreover, two transformations of the body can be conveniently composed. Let us consider three distinct configurations $A$, $B$ and $C$ of the rigid body (Fig. 2.4). The transformation from $A$ to $B$ and from $B$ to $C$ are respectively denoted $\mathbf{H}_{AB}$ and $\mathbf{H}_{BC}$. The configuration transformation from $A$ to $C$ is simplistically defined by the following composition law

$$
\mathbf{H}_{AC} = \mathbf{H}_{AB}\mathbf{H}_{BC}.
$$

(2.30)

The set $\mathcal{H}(\mathbf{R}, \mathbf{x})$ has the mathematical structure of a matrix Lie group, which is denoted as the special Euclidean group $SE(3)$. In this thesis, the Special Euclidean group $SE(3)$ is considered since this Lie group leads to a formalism with inherent valuable properties to perform the structural optimization of MBS.

**Lie group description of mechanical systems on $SE(3)$**

While continuing with a nonlinear finite element approach as in Géradin and Cardona (2001), the dynamics of flexible MBS can alternatively be described on a $k$-dimensional manifold $G$ with a Lie group structure (Brüls et al., 2012; Sonneville and Brüls, 2014; Sonneville et al., 2014). From a mathematical point of view, a Lie group $G$ is a differentiable manifold for which the product (or composition) and inversion operations are smooth maps and on which differential geometry can be employed to perform operations. This section briefly introduces some fundamentals of the Lie group theory. A more detailed description can be found in Holm et al. (2009) or Boothby (2009).

With the Special Euclidean group $SE(3)$, the configuration space $G$ of a flexible MBS is described as a set of frame transformations that can be represented by $4 \times 4$ matrices, defined as

$$
\mathbf{H}_I = \begin{bmatrix} \mathbf{R}_I & \mathbf{x}_I \\ 0_{3\times1} & 1 \end{bmatrix}.
$$

(2.31)

where $\mathbf{R}_I \in SO(3)$ is a rotation matrix and $\mathbf{x}_I \in \mathbb{R}^3$ is a position vector. These frames are used to describe 2 different features. 1) The absolute position and orientation of each node of the rigid and flexible bodies. 2) The relative transformation occurring in kinematic joints. As a consequence, a mixed variable formulation is achieved since absolute and relative variables are similarly treated. The matrix $\mathbf{H}_I$ has $k_I = 6$ degrees of freedom for each node of the rigid and flexible bodies, namely 3 translations and 3 rotations. However, for kinematic joints, the matrix $\mathbf{H}_I$ is restricted to belong to a subgroup of $SE(3)$ and has $k_I < 6$ degrees of freedom. Hence, the dimension $k$ of the group is obtained by summing the degrees of freedom of the nodes and the degrees
of freedom of the relative transformations. The configuration of the system $H$ is thus represented as a block diagonal matrix gathering all the $H_i$’s.

The composition operation $G \times G \rightarrow G$ that associates two elements of the group to one element of the group is based on the matrix product

$$H_{tot} = H_1 H_2.$$  \hspace{1cm} (2.32)

This composition rule has several properties, e.g. the existence of a neutral element $e$ such that $He = eH = H$, which is simply the identity matrix, and the existence of an inverse such that $\exists H^{-1} : HH^{-1} = H^{-1}H = e, \forall H \in G$.

The tangent space at a point $H \in G$ is a vector space denoted $T_H G$ and the Lie algebra is defined as the tangent space at the identity element of the group, i.e. $\mathfrak{g} = T_e G$. The Lie algebra is a vector space that is isomorphic to $\mathbb{R}^k$ by an invertible linear mapping,

$$\tilde{\cdot} : \mathbb{R}^k \rightarrow \mathfrak{g}, \, v \mapsto \tilde{v}.$$  \hspace{1cm} (2.33)

The time derivative can be introduced by mean of a left invariant vector field as

$$\dot{H} = H \tilde{v}$$  \hspace{1cm} (2.34)

where $\tilde{v}$ is an element of the Lie algebra $\mathfrak{g}$. This results from a fundamental property stating that a tangent vector at any point $H$ can be represented in the Lie algebra using the left translation map $L_H$. Indeed, $L_H$ is a diffeomorphism of $G$

$$L_H : G \rightarrow G, \, y \rightarrow Hy$$  \hspace{1cm} (2.35)

where $y \in G$ and its derivative define a diffeomorphism between $T_y G$ and $T_{Hy} G$. In the particular case $y = e$, a bijection exists between $T_e G = \mathfrak{g}$ and $T_H G$:

$$DL_H(e) : \mathfrak{g} \rightarrow T_H G, \tilde{w} \mapsto DL_H(e) \tilde{w}$$  \hspace{1cm} (2.36)

where $DL_H(e)\tilde{w}$ is the directional derivative of $L_H$ evaluated at point $e$ in the direction $\tilde{w} \in \mathfrak{g}$. Hence, a tangent vector $\tilde{w} \in \mathfrak{g}$ defines a left invariant vector field on $G$ which is constructed by the left translation of $\tilde{w}$ to the tangent space at any point of $G$.

At the light of the the previous developments, the Lie algebra is thus a vector space such that $\tilde{v}$ can be associated to a velocity vector $v$ of dimension $k$, which includes $6$ (resp. $k_I$) velocity variables for each node (resp. relative transformation). For each node, the element $\tilde{v}_I$ is defined as

$$\tilde{v}_I = \begin{bmatrix} \Omega_I & u_I \\ 0 & 0 \end{bmatrix}$$  \hspace{1cm} (2.37)
where \( \mathbf{u}_I \) corresponds to the 3 linear velocity component vector and \( \tilde{\Omega}_I \) is the well-known skew-symmetric matrix composed of the 3 angular velocity components

\[
\tilde{\Omega} = \begin{bmatrix}
0 & -\Omega_{I3} & \Omega_{I2} \\
\Omega_{I3} & 0 & -\Omega_{I1} \\
-\Omega_{I2} & \Omega_{I1} & 0
\end{bmatrix},
\]

(2.38)

The velocity vector \( \mathbf{v}_I \) represents the absolute velocity of a node expressed in the nodal local frame. Hence, the interpretation of the velocity vector is the same as with the classical nonlinear finite element approach.

The exponential map is a useful operator that maps any element of the Lie algebra to an element of the Lie group,

\[
\exp : \mathfrak{g} \to G, \tilde{\mathbf{q}} \mapsto \mathbf{q} = \exp(\tilde{\mathbf{q}}).
\]

(2.39)

The inverse map is called the logarithmic map,

\[
\log : G \to \mathfrak{g}, \mathbf{q} \mapsto \tilde{\mathbf{q}} = \log(\mathbf{q}).
\]

(2.40)

The nodal variables are \textit{a priori} considered as independent variables whereupon 6 kinematic constraints between nodal frames and relative transformation frames are introduced for each kinematic joint. Formally, \( m \) constraints \( \Phi : G \to \mathbb{R}^m \) are enforced, restraining the dynamics to the submanifold \( N \) of dimension \( k - m \)

\[
N = \{ \mathbf{H} \in G : \Phi(\mathbf{H}) = 0 \}.
\]

(2.41)

Equations of motion in a Lie group formalism

Using the classical principles of mechanics (Gérardin and Cardona, 2001) and following a similar approach as detailed in Section 2.1.3, the equations of motion of a flexible MBS described with a Lie group formalism on the Special Euclidean group \( SE(3) \) have the following index-3 differential-algebraic (DAE) structure

\[
\dot{\mathbf{H}} = \mathbf{H}\dot{\mathbf{v}}
\]

(2.42)

\[
\mathbf{r} = \mathbf{M}\dot{\mathbf{v}} - \dot{\mathbf{v}}^T\mathbf{Mv} + \mathbf{g}(\mathbf{H}) + \mathbf{B}^T(\mathbf{H})\mathbf{\lambda} = 0_{k \times 1}
\]

(2.43)

\[
\Phi(\mathbf{H}) = 0_{m \times 1}.
\]

(2.44)

where \( \dot{\mathbf{v}}(\bullet) \) is a linear operator of the Lie group which transforms a \( k \times 1 \) vector into a \( k \times k \) matrix (Brüls et al., 2011a). The configuration of the system is represented by \( \mathbf{H} \in G \), \( \mathbf{v} \in \mathbb{R}^k \) is the velocity vector and \( \mathbf{\lambda} \in \mathbb{R}^m \) is the vector of Lagrange multipliers associated with the constraints \( \Phi \). \( \mathbf{M} \) is the \( k \times k \) symmetric mass matrix, the vector \( \mathbf{g} \) gathers the external, internal and complementary inertia forces and \( \mathbf{B} \) is the \( m \times k \) matrix of constraint gradients.
Notice that the first equation is a matrix equation while the other two are vector equations. The equations of motion (2.42)-(2.44) represent the dynamics of a general class of conservative flexible multibody systems in a local frame approach. The formulation can be easily extended to account for non-conservative forces. More details about the derivation of the equations of motion are given in Article [4].

These equations of motion can be directly integrated on the nonlinear manifold without introducing generalized coordinates, i.e. without introducing a parameterization of rotations. The adopted Lie group time integrator described in Brüls and Cardona (2010) and in Brüls et al. (2012), is an extension of the generalized-$\alpha$ time integration method for the simulation of flexible multibody systems. This Lie group time integrator exhibits second-order accuracy for all solution components, i.e. for nodal translations, rotations and Lagrange multipliers.

The Lie group formalism offers several advantages compared to a classical nonlinear finite element approach. Firstly, no parameterization of rotations is needed to derive the equations of motion that can then be directly solved on the nonlinear manifold. It ensues important simplifications in the formulations and algorithms. Secondly, displacements and rotations are represented as increments with respect to the previous configuration, and those increments can be expressed in the local frame. As a result, geometric nonlinearities are automatically filtered from the relationship between incremental displacements and elastic forces, which strongly reduces the fluctuations of the iteration matrix during the simulation. The increments result from the Newton-Raphson iterative scheme that is used at each time step to satisfy the residual form of the equations of motion. The iterative process is similar to the one described for a standard nonlinear finite element formalism, see Equations (2.20)-(2.24). Furthermore, the choice of the Special Euclidean group $SE(3)$ combined with the left invariant representation of derivatives defined in Equation (2.36), enable to consider the tangent stiffness matrix $K_t$ as constant under the assumption of small deformations. The tangent stiffness matrix is defined from the directional derivative as $D_{r(H,v,\dot{v},\lambda)}\cdot\delta h = K_t\delta h$. The efficient evaluation of ESL for MBS optimization, as detailed in Article [4], takes advantage of these properties.

### 2.2 Structural optimization

This section introduces the fundamental principles of structural optimization and gives an overview of the techniques used in this work. In Chapter 3, these structural optimization techniques are coupled with the dynamic analysis of MBS to perform the structural optimization of MBS components.

#### 2.2.1 Design parameterizations and design variables

Over years, optimization techniques have been developed to improve the design process and to lessen the empirical or intuitive choices of the designer. The generality of
optimization methods is related to the number of inputs coming from the designer. Indeed, a smaller number of inputs leads to a broader design space and more freedom for the optimizer. Nevertheless a more general optimization problem usually requires a higher computational cost, which explains the concurrent evolution of optimization techniques and computational performance.

![Initial designs](image1)
![Optimal designs](image2)

Figure 2.5: Structural optimization parameterizations.

**Optimal sizing** of structures, also known as automatic sizing, is the simplest strategy in structural optimization. This method mainly concerns the modifications of transverse dimensions of structural components, such as the cross section of bars and beams or the thickness of plate and shell elements (Fig. 2.5), considering that the shape and the connectivity of the structure are known *a priori* and fixed during the optimization process. Since no geometrical modification of the structure arises, the same structural model, e.g. the finite element mesh, is kept along the optimization process.

Zienkiewicz and Campbell (1973) initiated the developments of *shape optimization* whereupon a rapid evolution occurred until reaching an industrial maturity. Shape optimization is a more ambitious method consisting in the design of internal and external boundaries of the structure without modifying the component topology. Two different approaches can be adopted. Firstly, the optimization problem can be formulated at the level of the CAD model, independently of the finite element model, wherein the design variables are the parameters describing the geometrical entities such as a length, a radius, etc, or more generally, the control points of NURBS curves (Braibant and Fleury, 1984; Beckers, 1991). Secondly, the shape optimization problem can accommodate the nodal coordinates and nodal thicknesses as design variables whereby the optimizer directly works on the finite element mesh (Bletzinger et al., 2010). Shape optimization is suitable to improve detailed design of structures considering simultaneously numerous criteria such as displacement, frequency, stress or buckling requirements.

The main issue of shape optimization concerns the mesh distortion occurring during the optimization. The regular mesh of the initial design is distorted after a few de-
Structural optimization

Sign iterations whereupon tangled and sliver elements appear. Ergo, the accuracy of the simulated response decreases. Adaptative mesh algorithms have been developed to combat this problem, however the re-meshing operations are time consuming (Haftka and Grandhi, 1986; Duysinx et al., 1994; Schleupen et al., 2000). Moreover, adapative mesh techniques produce discontinuities at the level of the discretized model and consequently in the objective function and/or constraints between iterations (Braibant and Morelle, 1990; Van Keulen et al., 2005).

Besides the classical shape optimization, Van Miegroet and Duysinx (2007) coupled a level set description of the geometry with the extended finite element method (X-FEM). This association leads to a generalized shape optimization wherein the component topology can be altered. More recently, Christiansen et al. (2015) combined shape and topology optimizations to perform 3D optimization of structures. Their optimization process is based on the Deformable Simplicial Complex (DSC) method (Misztal and Bærentzen, 2012), which represents a solid structure using a conforming tetrahedral mesh.

**Topology optimization** has been developed to determine the optimal design of a component without *a priori* information of the component layout (Bendsøe and Sigmund, 2003; Eschenauer and Olhoff, 2001). The optimization method only requires the definitions of the spatial design domain, material properties, boundary conditions and load cases. Hence, regarding the reduction of the cost function, this method outperforms the two previous methods for which the designer’s initial choices strongly influence the outcome of the optimization process.

As depicted in Figure 2.6, topology optimization problems can be formulated as an optimal distribution of a certain quantity of material within a fixed design domain in order to minimize some performance criteria, generally a global criterion such as the compliance or the fundamental eigenfrequency (Bendsøe, 1989). As a consequence, the explicit CAD design parameterization used in sizing and shape optimizations is replaced by an implicit representation. Two main parameterization approaches can be adopted either by using an indicator function leading to the SIMP approach (Bendsøe and Sigmund, 1999, 2003) or by resorting to level set functions (Wang et al., 2003; Allaire et al., 2004). Besides, topology optimization works on a fixed mesh avoiding the mesh distortion issues encountered in shape optimization.

Since the seminal work of Bendsøe and Kikuchi (1988) who first handled efficiently topology optimization using the homogenization method, this method has undergone considerable developments leading to an industrial maturity and the commercialization of several finite element codes, e.g. Optistruct by Altair\(^5\), Topol by Samtech\(^6\) and SIMULIA Tosca Structure by FE Design\(^7\), now owned by Dassault Systèmes.

\(^5\)www.altairhyperworks.com
\(^6\)www.plm.automation.siemens.com
\(^7\)www.fe-design.de
2.2.2 Design problem formulation

Engineering design problems can be cast into mathematical optimization problems upon which optimization methods can be applied. The optimization problem concerns the minimization of an objective function \( f_0(p) \) subjected to \( m \) constraints \( f_j(p) \leq \overline{f}_j \) which ensure the integrity of the structural design and its manufacturability (Haftka and Gürdal, 1992; Boyd and Vandenberghe, 2004; Nocedal and Wright, 2006). The vector \( p \) gathers the \( n_v \) independent design variables \( p_i \) that are modified by the optimizer. Side-constraints \( p_l \leq p_i \leq p_\overline{u} \) limit the design space and reflect technological considerations. Mathematically, the optimization problem reads

\[
\begin{align*}
\text{minimize} & \quad f_0(p) \\
\text{subject to} & \quad f_j(p) \leq \overline{f}_j, \quad j = 1, \ldots, m, \\
& \quad p_l \leq p_i \leq p_\overline{u}, \quad i = 1, \ldots, n_v.
\end{align*}
\] (2.45)

Depending on the type of optimization considered, the design variables \( p \) can be geometrical parameters of CAD features such as the radius of a circle or the position of NURBS curve control points for shape optimization or in topology optimization, they are related to the volume fraction of each element. The cost and constraint functions \( f_0 \) and \( f_j \) are generally implicit nonlinear functions of the design variables. They represent the mass, the compliance, the displacements, the stresses, etc.

With the general and robust design framework provided by this problem formulation, optimization problems can be solved using the various types of optimization algorithms presented in the next section.
2.2 Structural optimization

2.2.3 Optimization methods

Several strategies can be adopted to solve optimization problems. The beginnings of structural optimization were essentially based on **Optimality Criteria (OC)** methods that use an iterative scheme based on the optimality conditions to reach the optimal solution. The optimality condition characterizes the optimal solution and its definition constitutes the starting point of the method. It can be rigorously derived from mathematical statement such as the Karush-Kuhn-Tucker (KKT) conditions or it can be intuitive as for the fully stressed design (FSD) criterion (Haftka and Gürdal, 1992), which is the most famous criterion. Afterwards, an iterative procedure that modifies the variables during the optimization must be adopted. Rigorous mathematical methods or heuristic procedures can be implemented to progress towards the optimality condition. The first rigorous optimality criterion method has been introduced by Prager and Taylor (1968). Later on, Fleury (1979b) demonstrated the usefulness of optimality criteria by establishing a relationship between optimality criteria and dual solution methods combined with approximation techniques. However, these methods are problem-dependent and are only convenient to solve a limited number of optimization problems. Moreover, a lack of convergence can be observed with no guarantee to reach the optimum solution (Ma et al., 1993).

**Mathematical Programming (MP)** methods consist in a second family of strategies relying on mathematical tools to reach an optimum solution. The steepest descent method is the simplest MP method that uses the information given by the gradient of the functions to improve the current solution. To minimize the value of the function $f_0$, this method characterizes the improved solution $\mathbf{p}^*$ at a given iteration by $\mathbf{p}^* = \mathbf{p} - l \nabla f_0$, where $l$ is the step length and $-\nabla f_0$ is the descent direction. This iterative process continues until a convergence criterion is achieved. Constrained optimization problems are usually tackled by a Lagrangian approach which allows accounting for the constraints in a convenient way.

In structural optimization, the problem is generally nonlinear and implicit with respect to the design variables. To solve these problems efficiently, the resolution of the original problem is circumvented by solving a sequence of approximated sub-problems, which is nowadays known as the **sequential convex programming** (Schmit, 1960; Fox, 1965; Fleury, 1973; Schmit and Farshi, 1974; Schmit and Miura, 1976; Schmit and Fleury, 1980). The sub-problems are explicit in the design variables whereupon they can be solved efficiently using mathematical programming algorithms. Each structural response is replaced by an explicit approximation, which is generally built to be convex and separable.

Besides these deterministic methods, a third strategy concerns the **heuristic methods** which include the evolutionary algorithms (Ashlock, 2006; Simon, 2013; Eiben and Smith, 2003). Many variants of evolutionary algorithms exist but the underlying idea behind all these techniques is similar. Given a population of individuals, the environ-
mental pressure causes natural selection whereupon a fitness of the population rises. Concretely, an initial random set of candidate solutions, i.e. elements of the design space, is selected and an abstract fitness measure is related to each candidate based on the cost function to minimize, the least the better. Based on this fitness, natural evolution is applied to the candidates. The better are chosen to seek the next generation, the worst disappear while recombination and/or mutation of candidates are also used to generate new candidates for the next generation and to maintain the possibility of exploring the full design space. This process is repeated until a convergence criterion is reached, e.g. a criterion on the cost function or a maximum number of iterations. These evolutionary methods generally require a large number of iterations and function evaluations to converge to an acceptable solution but they suffer less from being stuck in local optima. These methods are useful when the gradient computations of the functions are painstaking or not available since these are zero-order methods. Swarm algorithms are related to this class of heuristic methods (Kennedy and Eberhart, 1995).

Many high-fidelity models are so computationally expensive that applying the previous optimization methods directly to the problem is not practical, often due to a time constraint. As a consequence, approximate models, also called surrogate models or meta models, are constructed whereupon the optimization is performed (Roux et al., 1998; Queipo et al., 2005; Myers et al., 2009; Colson et al., 2010; Koziel and Leifsson, 2013). Classical and popular surrogate models are polynomial response surfaces, Kriging, support vector machines and artificial neural networks. During the optimization process, a correction may be applied to the approximate model so that it better fits the original model. Different corrections were developed such as the additive/multiplicative correction (Eldred et al., 2004), the space mapping (Bandler et al., 1994, 2004) and the manifold mapping (Echeverria and Henker, 2005).

2.2.4 Mathematical programming approach

Mathematical programming approach is mainly adopted in this thesis. Therein, this section details its main principles.

Concepts of approximations and convex sub-problems

The general optimization problem (2.45) generally involves nonlinear and implicit functions with respect to the design variables. Furthermore, their nature results in a monotonous or non-monotonous behavior with respect to a given design variable change. Hence, the direct solution of the original problem with mathematical programming methods is too heavy from a computational point of view since the evaluation of the functions and their derivatives require a numerical computation, e.g. finite element analysis or MBS analysis. In order to solve efficiently the problem, Fleury (1973) proposed to replace the resolution of the original optimization problem (2.45) by a sequence of explicit sub-problems (2.46) with respect to the design variables, that are
solved iteratively. The approximated problem reads

$$\begin{align*}
\text{minimize} \quad & \tilde{f}_0^k (p) \\
\text{subject to} \quad & \tilde{f}_j^k (p) \leq f_j, \quad j = 1, \ldots, m, \\
& p_i - \alpha_i^k \leq p_i \leq p_i + \beta_i^k, \quad i = 1, \ldots, n_v.
\end{align*}$$

(2.46)

where $k$ is the iteration number, $\tilde{\cdots}$ denotes the explicit approximation of the functions around the current design point $p^{(k)}$ and the parameters $\alpha_i^k$ and $\beta_i^k$ are move limits that restrain the modification of the current design point within a neighborhood. The idea underlying the method is that each sub-problem must steadily improve the solution of the original problem and converge towards the original problem, i.e. a convergent series of design points.

Later on, the notion of **sequential convex programming** (SCP) generalized the approach wherein each approximation is convex to enforce a conservative behavior (Fleury, 1993). As illustrated in Figure 2.7, an explicit approximation is constructed at the current design using an expansion based on the value of the responses, combined with their first order derivatives and sometimes also with their second order derivatives. Afterwards, efficient mathematical programming algorithms such as Lagrangian maximization (dual method) or interior point methods are used to solve the approximated problems. The iterative process of the SCP method is illustrated in Figure 2.8.

![Sequential convex programming approach](image)

**Figure 2.7:** Sequential convex programming approach.

**Resolution of the approximated sub-problems**

The idea of replacing the original problem by a sequence of sub-problems stands since efficient mathematical programming algorithms exist to solve the sub-problems. Indeed, powerful and efficient methods such as sequential quadratic programming (SQP) methods (Belegundu and Arora, 1984; Schittkowski, 1986) are tailored to solve these types of problems. Nonetheless, the demonstration of obtaining an efficient method has been realized by Fleury (1979a) who proposed to resort to a dual maximization...
Initialization: $k = 0$ and initial design $p^{(k)}$ 

At the current point $p^{(k)}$, computation of the cost and constraint function responses and their derivatives:

$$f_j(p^{(k)}) \quad \text{and} \quad \frac{\partial f_j(p^{(k)})}{\partial p_i}, \quad j = 0, \ldots, m \quad \text{and} \quad i = 1, \ldots, n_v$$

Generation of the approximated functions:

$$\tilde{f}_j(p), \quad j = 0, \ldots, m$$

Resolution of the explicit sub-problem. Then $p^{(k+1)} = p^{(k)*}$ and $k = k + 1$.

Convergence?

Yes

Stop

No

Figure 2.8: Iterative process of the sequential convex programming method (Bruyneel et al., 2002).

The dual approach. In this approach, the primal problem with a high number of variables is replaced by its dual problem. In the dual space of the Lagrange multipliers associated to the constraints, the optimization problem is transformed into a quasi-unconstrained maximization problem of the dual function. The effectiveness of the method lies in the dimension of the problem which is limited to a sub-space related to the set of active constraints. Thusly, the effectiveness of the method is conditioned by a high ratio between the number of design variables and the active constraints, making the dual space dimension much smaller than the primal space dimension. Furthermore, the dual approach is even more appealing if the approximated sub-problem is convex and separable because the primal-dual relationships are not expensive.

Adopting high quality approximations that have been developed over years (see next section), the most efficient approach combines dual and SQP concepts. In this approach, the primal or dual sub-problems are also solved using a sequence of quadratic sub-problems (Fleury, 1993).
Approximation schemes

The key element of the sequential convex programming approach lies in the quality of the approximation with the smallest cost of information evaluation to build it. These approximations must be explicit for each function, they must be convex to have a conservative behavior and to allow a dual solution as well as being separable to obtain low-cost primal-dual relationships. Several types of approximation schemes have been proposed in the literature. The most famous are hereafter reviewed. Depending on the approximation schemes, several efficient optimization algorithms have been proposed such as SQP (Schittkowski, 1986), ConLin (Fleury, 1989a), MMA (Svanberg, 1987), GCMMA (Svanberg, 2002) and some extended versions of MMA (Bruyneel et al., 2002).

First order and monotonous approximation

The ConLin scheme developed by Fleury and Braibant (1986) is a convex approximation based on a first-order Taylor series expansion with respect to either direct or reciprocal variables. Using both types of design variables is necessary to generate approximations whose curvature is strictly positive or null. The algorithm selects a linearization in terms of direct and reciprocal design variables upon the sign of the derivatives.

The approximation of a design function \( \tilde{f}_j(p) \) is expressed based on the function response and on the first derivatives at the current design point \( p^{(k)} \) as

\[
\tilde{f}_j(p) = f_j|_{p^{(k)}} + \sum_{+,i} \frac{\partial f_j}{\partial p_i} \bigg|_{p^{(k)}} (p_i - p_i^{(k)}) \\
- \sum_{-,i} \left( p_i^{(k)} \right)^2 \frac{\partial f_j}{\partial p_i} \bigg|_{p^{(k)}} \left( \frac{1}{p_i} - \frac{1}{p_i^{(k)}} \right)
\]  

(2.47)

where the symbols \( \sum_{+,i} \) and \( \sum_{-,i} \) denote the summations over terms having positive and negative first-order derivatives, respectively. Since this linearization scheme only provides convex and separable approximations, Fleury and Braibant (1986) suggested the name ConLin for “Convex Linearization”. Furthermore, since the created subproblems are convex and separable, a dual approach is particularly suitable. Starnes Jr. and Haftka (1979) demonstrated that this scheme leads to the most convex approximation that can be created using a combination of mixed variables.

In some circumstances, the ConLin scheme may be penalized due to an inadequacy between the real curvature and its approximation. If the curvature is too low, oscillations appear in the convergence process while a too high curvature slows down the convergence rate. Furthermore, the curvature depends on the sign of the derivative and varies with the design variable. It is also noted that the second derivative of the approximations are fixed and can not be modified.
Following these drawbacks, Svanberg (1987) proposed a generalization of the approach leading to the Method of Moving Asymptotes (MMA). Looking back, the ConLin scheme can be interpreted as if the inverse linearization considers a vertical asymptote in \( p = 0 \) while the direct linearization positions a vertical asymptote at \( p = +\infty \). Therein, the MMA method introduces vertical asymptotes in the approximation expression, whose positions can be adapted. Indeed, by modifying the position of the asymptotes with respect to the design point, it is possible to better fit the curvature of the real problem, i.e. the method enables to adjust the convexity of the approximation.

In the MMA method, each function is approximated using two types of intermediate variables \( \frac{1}{U_i^{(k)} - p_i} \) and \( \frac{1}{p_i - L_i^{(k)}} \) that leads to

\[
\tilde{f}_j(p) = f_{0j} + \sum_{i=1}^{n} \frac{r_{ij}^{(k)}}{U_i^{(k)} - p_i} + \sum_{i=1}^{n} \frac{q_{ij}^{(k)}}{p_i - L_i^{(k)}} \quad (2.48)
\]

where the parameters \( U_i \) and \( L_i \) define the asymptotes related to the design variable \( p_i \), and satisfy the criterion \( L_i \leq p_i \leq U_i \). In Equation (2.48), only one of the two coefficients \( r_{ij}^{(k)} \) or \( q_{ij}^{(k)} \) is different from zero at the same time for one design variable.

Furthermore, the values of \( r_{ij}^{(k)} \), \( q_{ij}^{(k)} \) and \( f_{0j} \) are adjusted in order to retrieve the function value and its derivatives from the approximation at \( p = p^{(k)} \). It yields

\[
r_{ij}^{(k)} = \max \left\{ 0, \left( U_i^{(k)} - p_i^{(k)} \right)^2 \frac{\partial f_j}{\partial p_i} \bigg|_{p^{(k)}} \right\}, \quad (2.49)
\]

\[
q_{ij}^{(k)} = \max \left\{ 0, -\left( p_i^{(k)} - L_i^{(k)} \right)^2 \frac{\partial f_j}{\partial p_i} \bigg|_{p^{(k)}} \right\}, \quad (2.50)
\]

\[
f_{0j} = f_j \big|_{p^{(k)}} - \sum_{i=1}^{n} \frac{r_{ij}^{(k)}}{U_i^{(k)} - p_i^{(k)}} - \sum_{i=1}^{n} \frac{q_{ij}^{(k)}}{p_i^{(k)} - L_i^{(k)}}. \quad (2.51)
\]

Depending on the sign of the first order derivative \( \frac{\partial f_j}{\partial p_i} \bigg|_{p^{(k)}} \), only one asymptote is used for each design variable \( p_i \). As a consequence, the approximation is always a monotonous function.

Deriving the approximation expression (2.48), it is observed that the approximation is a monotonous increasing or decreasing function and that the second order derivatives at \( p = p^{(k)} \) read

\[
\frac{\partial^2 \tilde{f}}{\partial p_i^2} \bigg|_{p^{(k)}} = -\frac{2}{\left( p_i^{(k)} - L_i^{(k)} \right)^2} \frac{\partial f_j}{\partial p_i} \bigg|_{p^{(k)}} \quad \text{or} \quad \frac{\partial^2 \tilde{f}}{\partial p_i^2} \bigg|_{p^{(k)}} = \frac{2}{\left( U_i^{(k)} - p_i^{(k)} \right)^2} \frac{\partial f_j}{\partial p_i} \bigg|_{p^{(k)}}. \quad (2.52)
\]

From these relations, it is obvious that the curvature increases if the asymptote gets nearer to the linearization point and decreases in the opposite case.

To update the asymptote parameters from one iteration to another, Svanberg (1987)
proposed a heuristic scheme. This scheme is based on the convergence history of the design variables and it reads

\[ \begin{align*}
L_i^{(k)} &= p_i^{(k)} - s_i \left( p_i^{(k-1)} - L_i^{(k-1)} \right), \\
U_i^{(k)} &= p_i^{(k)} + s_i \left( U_i^{(k-1)} - p_i^{(k-1)} \right)
\end{align*} \]

(2.53)

(2.54)

where the parameter \( s_i \) is computed based on the variation of the corresponding design variable values \( p_i \) within three iteration steps.

It is worth noticing that the process defines a pair of asymptotes for each variable but it uses the same asymptotes for all the functions. In order to adjust the level of convexity for each function independently, some researchers generalized the classical MMA method by attaching a proper set of moving asymptotes to each design variable for each design function, i.e. \( L_i^{(k)} \) or \( U_i^{(k)} \) are replaced by \( L_{ij}^{(k)} \) or \( U_{ij}^{(k)} \). The resulting method is named the Generalized Method of Moving Asymptotes (GMMA).

**First order and non-monotonous approximation**

In order to create non-monotonous approximations, Svanberg (1995) proposed to extend the MMA approximation scheme (2.48) in which both \( r_{ij} \) and \( q_{ij} \) become simultaneously nonzero. Therein, both asymptotes are used to create the approximation and defer to it the non-monotonous behavior. Furthermore, a term associated to a non-monotonic parameter \( \rho_j^{(k)} \) is introduced in the definition of \( r_{ij} \) and \( q_{ij} \). By updating the non-monotonic parameter and the asymptotes according to the rules given by Svanberg (1995), the global convergence property of the approximation scheme can be proven, which leads to the globally convergent version of MMA (GCMMA). More details can be found in Svanberg (1995) and Svanberg (2002).

**Second order and non-monotonous approximation**

A second order approximation of a function \( f_j \) is straightforwardly achieved by employing a Taylor series expansion around the design point and limited at the second order, leading to

\[ \tilde{f}_j (p) = f_j_{\mid p^{(k)}} + (p - p^{(k)})^T \nabla f_j_{\mid p^{(k)}} + \frac{1}{2} (p - p^{(k)})^T \nabla^2 f_j_{\mid p^{(k)}} (p - p^{(k)}) \]

(2.55)

where \( \nabla f_j \) is the gradient of \( f_j \) and \( \nabla^2 f_j \) is the Hessian matrix of \( f_j \). The approximation is not separable since second order cross derivatives are involved.

In order to solve the constraint optimization problem, a Newton iterative scheme combined with the Lagrangian function of the optimization problem and the Karush-Kuhn-Tucker conditions are used. Moreover, convergence of the procedure can be guaranteed
Several other variants of the SQP algorithm solve the constraint optimization problem, e.g. the most famous are from Han (1976), Han (1977), Pshenichny and Danilin (1978), Schittkowski (1981) and Schittkowski (1986).

The bottleneck of this approach lies in the evaluation of the second order derivatives that become extremely costly when the number of design variables grows since \( i(i + 1)/2 \) evaluations. Furthermore, the dual approach is not efficient since the approximation is not separable as noted previously. Ergo, Fleury (1989c) suggested to only consider the diagonal terms of the Hessian matrix and to neglect the effects of the cross derivatives. The quadratic separable approximation reads

\[
\tilde{f}_j(p) = f_j(p^{(k)}) + \sum_{i=1}^{n} \frac{\partial f_j}{\partial p_i}(p^{(k)}) (p_i - p_i^{(k)}) + \frac{1}{2} \sum_{i=1}^{n} \left( \frac{\partial^2 f_j}{\partial p_i^2}(p^{(k)}) + \delta_{ii} \right) (p_i - p_i^{(k)})^2 \quad (2.56)
\]

where the terms \( \delta_{ii} \) are added to easily adjust the convexity behavior of the approximation. This expression gave rise to the diagonal SQP algorithm.

### 2.2.5 Sensitivity analysis

Gradient-based optimization methods require a sensitivity analysis to compute the derivatives of the structural responses, i.e. the functions \( f_j \), with respect to the design variables. The sensitivities are provided to the optimizer to build accurate approximations of the problem and to determine effective descent directions. The efficiency of the sensitivity analysis is essential in the optimization process because it can drastically affect the computation time, especially when the simulation time is large.

Let us consider a general response function \( f_j \) representing any performance measure or restriction within the optimization problem. The function \( f_j \) has the general form

\[
f_j = f_j(p, q(p)) \quad (2.57)
\]

where \( q \) is the solution of the equilibrium equation. The function \( f_j \) depends explicitly on the design variables \( p \) and implicitly through the structural response \( q \). Therein, invoking the chain rule, the total derivative of the function \( f_j \) with respect to the design variable \( p_i \) reads

\[
\frac{df_j}{dp_i} = \frac{\partial f_j}{\partial p_i} + \frac{\partial f_j}{\partial q} \frac{dq}{dp_i}. \quad (2.58)
\]

In contrast to the derivatives of the first two terms \( \partial f_j/\partial p_i \) and \( \partial f_j/\partial q \), that are easily calculated since the functions \( f_j \) depends explicitly on \( p_i \) and \( q \) respectively, the derivative of the term \( dq/dp_i \) is more difficult to compute. Indeed, the structural response \( q \) depends implicitly on \( p_i \) through the equilibrium equation and so do its derivatives. To compute the sensitivities, several methods can be used and they are hereafter described.
Finite difference method

Finite difference sensitivity analysis method is undoubtedly the most simple approach. The total derivative of the function $f_j$ is approximated using a Taylor series expansion. Three forms of finite difference are commonly used. Forward (2.59) and backward differences are the most used with a truncation error of $O(\Delta p_i)$. As a consequence, a smaller $\Delta p_i$ yields a more accurate approximation. Nonetheless, a too small $\Delta p_i$ deteriorates the accuracy of the computation since numerical round-off errors appear (Greene and Haftka, 1991). Central differences (2.60) are used to achieve a better accuracy with a truncation error of $O(\Delta p_i^2)$.

$$
\frac{df_j}{dp_i} \approx \frac{\Delta f_j}{\Delta p_i} = \frac{f_j(p + \Delta p_i) - f_j(p)}{\Delta p_i}, \quad (2.59)
$$

$$
\frac{df_j}{dp_i} \approx \frac{\Delta f_j}{\Delta p_i} = \frac{f_j(p + \Delta p_i) - f_j(p - \Delta p_i)}{2\Delta p_i}, \quad (2.60)
$$

where $\Delta p_i = [0 \ldots 0, \Delta p_i, 0 \ldots 0]$ is the parameter perturbation.

Finite difference methods are easy to implement and can accommodate almost any type of functions. Nevertheless they suffer from computational inefficiency since they require at least one additional simulation per design variable and therefore, the CPU cost grows by a factor $n_v + 1$, where $n_v$ numbers the design parameters. Furthermore, this method suffers from two types of errors: truncation and round-off errors that lead to a difference between the numerical evaluation of the function and its exact value (Moin, 2010; Tortorelli and Michaleris, 1994). Truncation errors, also known as discretization errors, occur with large perturbation steps leaving from the small perturbation assumption. The round-off errors concern the loss of precision due to computer rounding of decimal quantities.

For these reasons, the finite difference method is viewed as a last resort for computing sensitivities while still being suitable to carry out investigations on a new problem.

Direct differentiation method

The direct differentiation method first evaluates the derivative $dq/dp_i$ and then computes the total derivative $df_j/dp_i$ (Tortorelli and Michaleris, 1994). The method begins by differentiating the equilibrium equation with respect to the design parameters $p$. Let us consider a linear static problem whose equilibrium equation is stated as

$$
K(p)q(p) = g(p). \quad (2.61)
$$

Differentiating Equation (2.61) yields

$$
\frac{dK}{dp_i}q + K\frac{dq}{dp_i} = \frac{dg}{dp_i} \quad (2.62)
$$
which can be rearranged as

\[ K \frac{dq}{dp_i} = \frac{dg}{dp_i} - \frac{dK}{dp_i} q. \] (2.63)

Solving the above *pseudo problem* gives the *pseudo response* \( dq/dp_i \) whereupon the total derivatives \( df_j/dp_i \) is obtained with Equation (2.58).

This method can be efficient if properly implemented. Indeed, Equation (2.63) resembles to the equilibrium equation (2.61). Hence, by storing the decomposed stiffness matrix \( K \) during the structural analysis, the derivatives \( dq/dp_i \) can be obtained in an inexpensive way by forming the *pseudo load* \( \frac{dg}{dp_i} - \frac{dK}{dp_i} q \) and then performing a backward substitution. This process is repeated for each design parameter \( p_i \).

In comparison with the finite difference method, the method is more efficient since it does not require additional stiffness matrix assemblies and decompositions for each design parameter perturbation. Moreover, these results are exact in the sense that they do not suffer from the truncation errors.

### Adjoint method

The adjoint method concerns the elimination of the derivative \( dq/dp_i \) from Equation (2.58) (Tortorelli and Michaleris, 1994). To this end, an augmented function \( \tilde{f}_j \) that incorporates the equilibrium equation (2.61), is defined via a Lagrange multiplier method and is stated as

\[ \tilde{f}_j = f_j(p, q(p)) - \lambda(p)(K(p)q(p) - g(p)) \] (2.64)

where \( \lambda \) is the Lagrange multiplier vector. Since the augmented term \( K(p)q(p) - g(p) \) equals zero, we have \( \tilde{f}_j = f_j \). Differentiating and rearranging the above equation yields

\[ \frac{d\tilde{f}_j}{dp_i} = \left( \frac{\partial f_j}{\partial p_i} - \lambda \left( \frac{dK}{dp_i} q - \frac{dg}{dp_i} \right) \right) + \frac{dq}{dp_i} \left( \frac{\partial f_j}{\partial q} - K^T \lambda \right) \] (2.65)

where the equilibrium equation (2.61) is used to simplify the expression. As the mechanical problem is a self adjoint problem, the stiffness matrix is symmetric \( K = K^T \). Since the Lagrange multiplier vector \( \lambda \) is arbitrary, it can be selected to annihilate the coefficient of the \( dq/dp_i \) term. As a result, the sensitivity expression gets rid of the unknown derivative \( dq/dp_i \).

To determine the *adjoint response* \( \lambda \), the following *adjoint problem* must be solved

\[ K^T \lambda = \frac{\partial f_j}{\partial q}. \] (2.66)

Once the *adjoint response* is computed, the desired sensitivity is obtained from the first term in parentheses of Equation (2.65). Indeed, considering the equilibrium equation, it is straightforward to establish that \( \frac{d\tilde{f}_j}{dp_i} = \frac{df_j}{dp_i} \).
2.2 Structural optimization

As for the direct differentiation, the new problem to solve has the same form as the equilibrium equation. Thusly, the *adjoint response* is efficiently computed by forming the *adjoint load* and performing a backward substitution into the already decomposed stiffness matrix. This method also avoids the truncation errors and results are efficiently obtained when compared to the finite difference method. The adjoint problem requires as many solutions of the adjoint problem as the number of response functions.

**Direct differentiation method vs adjoint method**

The direct differentiation method and the adjoint method are employed to compute the same term but their purpose is different. The computational cost is similar. Both require evaluating a pseudo load and then solving an associated problem using backward substitutions. However, the adjoint method requires to solve one adjoint problem for each response function $f_j$, whereas the direct differentiation method requires to solve one pseudo problem for each design parameters $p_i$. As a consequence, the adjoint method is preferred when the number of response functions is smaller than the number of design parameters. In the opposite case, the direct differentiation method is preferable.
Chapter 3

Structural optimization of flexible components within a MBS approach

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This chapter presents the different approaches and methods employed to perform the structural optimization of MBS components. Concurrently to the introduction of the different research topics, the major results of the work are pointed out. Based on the accumulated experience, the two main optimization methods are discussed.
3.1 Introduction

The structural optimization of flexible components within a MBS involves the coupling of several software tools. A general flowchart of the coupling approach is illustrated in Figure 3.1. As observed, several complementary software packages are involved in the optimization process. The process starts with the creation of a geometrical model representing the physical system. Afterwards, before running the MBS simulation, a mesh generator is often used to introduce flexibility via the finite element method within the MBS analysis. With a nonlinear finite element program, these last two steps are integrated since the flexibility stems naturally from the formulation. Finally, the optimization process, gathering the sensitivity analysis and the numerical optimization, is in charge of generating an improved design to close the loop. Afterwards, the process is restarted until a satisfactory design is obtained.

Figure 3.1: MBS optimization flowchart.

The coupling of these software tools may restrict the designer’s freedom, especially when using commercial software tools. The limitations mainly arise from the information exchanges that must occur between the different software packages. For instance, to perform an efficient sensitivity analysis using semi-analytical methods, one needs to get access to the data coming from the MBS simulation and these are usually rather complex to extract. In order to obtain an efficient coupling, a monolithic approach wherein all the tools are embedded is appealing. However, it relies on the companies owning the software tools, i.e. they have to enable communications with their software tools. Another possibility is to use open data structures and open solvers allowing the access and the treatment of the data.

These limitations have already been encountered in multidisciplinary optimization where thorny problems are faced concerning the integration of several software pack-
Component parameterization using a level set description

3.2 Component parameterization using a level set description

3.2.1 From explicit to implicit representation of the geometry

In shape optimization, the component geometry is generally described explicitly, e.g. using circles, splines, etc. This explicit representation hinders deep modifications of the component geometry such as topological changes and is partly responsible for the moderate performance improvement in classical shape optimization (Haftka and Grandhi, 1986). In contrast to topology optimization, the explicit representation using CAD entities permits to keep smooth and well-defined boundaries that are not subject to interpretations. Moreover, well-defined models allow an accurate computation of the system response.

In this work, the level set description of the component geometry is the cornerstone of an extended method laying in between shape and topology optimizations, namely the Generalized Shape Optimization Method (Van Miegroet and Duysinx, 2007). The level set description consists in an implicit representation of the component geometry whereby the advantages of both optimization methods can be combined. Firstly, the component geometry is precisely described by CAD entities with a reasonable number
Chapter 3. Structural optimization of flexible components within a MBS approach

of parameters as in shape optimization. Secondly, the geometrical description works with a fixed mesh grid which avoids the mesh management difficulties presented in Section 2.2.1. Thirdly, the component topology can be changed in a limited manner.

Originally, the level set method was developed as a numerical technique for tracking interfaces and shapes. It was introduced by Osher and Sethian (1988) who suggested an implicit representation to facilitate the tracking of an interface instead of the traditional explicit method. The implicit description relies on the introduction of a smooth scalar-valued function \( \phi \), namely the level set function (LSF), which is mathematically defined as

\[
\phi : D \in \mathbb{R}^n \times \mathbb{R}^{n_v} \rightarrow \mathbb{R}
\]

(3.1)

where \( D \in \mathbb{R}^n \) is the design domain (\( D \in \mathbb{R}^2 \) for planar geometry and \( D \in \mathbb{R}^3 \) for 3D geometry) and \( \mathbb{R}^{n_v} \) is the parameter space. The boundary \( \Gamma \) is subsequently represented by the set of dimension \( n - 1 \)

\[
\Gamma = \{(x, p) \in D \times \mathbb{R}^{n_v} : \phi(x, p) = 0\}
\]

(3.2)

where \( x \) is an element of the design domain \( D \) and \( p \) is the design parameter vector. Hence, the boundary is implicitly defined as the zero-level of a higher dimension scalar function, i.e. the LSF \( \phi(x, p) \). Likewise, working with solid-void structures, the LSF defines the material domain \( \Omega \), the void domain \( D \setminus \Omega \) and the material interface \( \partial \Omega \) as

\[
\begin{cases}
\phi(x, p) > 0, & \iff x \in \Omega \text{ (material)} \\
\phi(x, p) < 0, & \iff x \in D \setminus \Omega \text{ (void)} \\
\phi(x, p) = 0, & \iff x \in \partial \Omega \text{ (interface)}.
\end{cases}
\]

(3.3)

During the optimization process, both shape and topology of the domain \( \Omega \) can be altered according to the changes of the LSF parameter \( p \).

To illustrate the level set description of geometries, let us introduce a hole in a \( 1 \times 1 \) m square plate. For simplicity’s sake, the LSF \( \phi(x) \) is defined by the analytical function of a super-ellipse that reads

\[
\phi(x) = \left| \frac{(x - c_x)}{a} \right|^{\xi} + \left| \frac{(y - c_y)}{b} \right|^{\eta} - 1.
\]

(3.4)

The level set function is illustrated in Figure 3.2 with the following set of parameters: \( a = 0.3 \) m, \( b = 0.2 \) m, \( c_x = c_y = 0.5 \) m and \( \xi = \eta = 3 \). In Figure 3.2(b), the isocontours are plotted and the boundary of the super-elliptical hole can be observed as the zero-level of the LSF.

3.2.2 Parameterization and mapping of the level set function

Numerous level set methods and approaches have been developed to perform structural optimization (Van Dijk et al., 2013). Therein, in order to categorize each method, the
3.2 Component parameterization using a level set description

(a) Level set function $\phi(x)$.  

(b) Isocontour representation of $\phi(x)$.  

Figure 3.2: Implicit representation of a super-ellipse feature.

authors recommend to mention the LSF parameterization and the geometry mapping, defining the link between the geometrical model and its mechanical counterpart.

In this thesis, the implicit representation of the geometry is combined with common CAD entities such as circles, splines, NURBS, etc. That is the LSF parameterization, based on CAD features, enables a precise description of the geometry. Analytical functions can be adopted for simple features. Nonetheless, using polar coordinates, Gielis (2003) introduced a Superformula $\phi_{sf}$, expressed as

$$\phi_{sf} = \frac{1}{\left( \left( \frac{1}{a} \cos \left( \frac{m}{4} \theta \right) \right)^{n_2} + \left( \frac{1}{b} \sin \left( \frac{m}{4} \theta \right) \right)^{n_3} \right)^{1/n_1}}$$

(3.5)

where $n_i, m \in \mathbb{R}^+$ and $a, b \in \mathbb{R}^+_0$. This function describes a large variety of shapes using a single and simple geometrical equation. Several features are illustrated in Figure 3.3. For more complex features, the signed-distance function $d(x)$ can be used, which is defined as

$$d(x) = \min_{x \in \Gamma} \|x - x_{\Gamma}\|, \quad \forall x \in D$$

(3.6)

where $\|\cdot\|$ denotes the Euclidean norm.

Each geometrical feature is described by a specific LSF although different LSF can describe the same geometrical feature (non-uniqueness). Afterwards, the final component geometry is generated by applying boolean operations to the individual features, i.e. the Constructive Solid Geometry approach is employed (Shapiro, 2007). The creation of a cross hole in a square plate using an union operator is illustrated in Figures 3.4(a)-3.4(c).
In this thesis, the flexible components of MBS are modeled using the finite element method. Therefore, the level set function geometry must be mapped to the finite element mesh. To do so, a volume fraction based Eulerian approach is adopted (Norato et al., 2004). The approach is similar to the SIMP in topology optimization wherein a pseudo density is assigned to each element depending on the number of nodes in $\Omega$ and in $D \setminus \Omega$. Allaire et al. (2004) also adopted a similar mapping wherein an Ersatz material is introduced for element laying across the boundaries. Figure 3.4(d) illustrates such a mapping on the cross hole example. More details about the adopted parameterization and geometry mapping are given in Article [2].

3.2.3 Implicit representation and structural optimization of MBS

The design problem of MBS components is nonlinear in essence since the MBS analysis is already nonlinear. Developing such an optimization problem parameterization aims at enabling deep modifications of the component geometry while keeping a compact design parameterization and thus a simple optimization process. It is known that the adopted geometry mapping leads to fuzzy boundaries regarding the finite element model. However, since the geometry is described by CAD features, the exact geometry is known. As a consequence, the manufacturability is straightforward. Moreover, this approach is interesting for industrial applications involving confidentiality. Indeed, the proprietary CAD model used to generate the initial model is not required for the optimization, only the finite element mesh must be shared.
3.2 Component parameterization using a level set description

(a) Implicit representation of a first super-ellipse feature.

(b) Implicit representation of a second super-ellipse feature.

(c) Exact geometry of the cross hole.

(d) Mapping resulting of the boolean operation $\text{AND}$ of the two LSF’s.

Figure 3.4: Geometrical description of a cross hole in a square plate.

It is worth noticing that the adopted implicit representation of the component geometry differs from a true topology optimization based on a level set approach (Wang et al., 2003; Allaire et al., 2002, 2004). Indeed, the number of holes in the geometry is introduced $a$ $priori$ so that topological changes are limited to holes merging. Hence, the optimal topology may be absent from the design space since holes cannot be nucleated. However, as a future extension, introducing the topological derivative (Novotny and Sokolowski, 2013) can remedy this limitation.

As an illustrative example, the optimization of a connecting rod presented in Article [2] is considered. The objective is to minimize its mass while restraining its elongation under operating conditions. Figure 3.5 illustrates the connecting rod geometry at different stages of the optimization process. It is observed that the geometry and especially the topology, i.e. the connectivity, continuously evolves as the optimization proceeds.
3.3 Fully coupled method

The fully coupled method relies on the optimization of the dynamic response coming directly from the MBS analysis. Therein, it involves dynamic response optimization problems that are rather challenging compared to classical structural optimization problems chiefly due to the difficulties of evaluating and considering the dynamic response in the optimization. In this section, the optimization process framework and the optimization problem formulation are first discussed. The difficult treatment of time-dependent constraints is then introduced and its impact over the optimization convergence is pointed out. Finally, the sensitivity analysis of MBS is revisited and the advantages of the proposed method are detailed.

3.3.1 Framework of the optimization process

The optimization problem is formulated as an extension of the optimization problem formulation (2.45) in which the time parameter \( t \) steps in, leading to a dynamic response optimization problem. Extending the formulation (2.45) and incorporating explicitly the equations of motion (2.9)-(2.10), expressed with a classical nonlinear finite element formalism, it comes

\[
\begin{align*}
\text{minimize} & \quad f_0 (s) \\
\text{subject to} & \quad M(q,p) \ddot{q} + g(q, \dot{q}, p) + \Phi_q^T(q,p) (k \lambda + p \Phi(q,p)) = 0, \\
& \quad k \Phi(q,p) = 0, \\
& \quad q(t_0) = q_0(p), \quad \dot{q}(t_0) = \dot{q}_0(p), \quad \forall t \in [t_i, t_f], \\
& \quad f_j(s,t) \leq f_j, \quad j = 1, \ldots, n_c, \\
& \quad p_i \leq p_i \leq p_i, \quad i = 1, \ldots, n_v.
\end{align*}
\]

(3.7)

The vector

\[
s = [q, \dot{q}, \ddot{q}, \lambda, p]
\]

(3.8)
gathers the dependent variables $\mathbf{q}, \dot{\mathbf{q}}, \ddot{\mathbf{q}}$ and $\lambda$, defining the MBS response and the vector of the $n_v$ independent design variables $\mathbf{p}$, ruling the optimization process. The first set of variables is denoted as “dependent” since they implicitly depend on the design variables $\mathbf{p}$. However, as a nested approach is used, they are not directly involved in the optimization process since they can be eliminated from the optimization problem after the forward time integration of the equations of motion. The time dependency of $\mathbf{q}, \dot{\mathbf{q}}, \ddot{\mathbf{q}}$ and $\lambda$ is not explicitly indicated for the sake of conciseness. We note that the optimization problem (3.7) is totally general and can incorporate equality constraints as well as functional constraints.

The flowchart of the fully coupled method process is provided in Figure 3.6. Using this method, the MBS simulation and the optimization process work in an integrated manner, i.e. a MBS analysis is performed at each iteration of the optimization and provides the sensitivities to the optimizer. The optimization process loops until a convergence criterion is achieved. As shown in Section 3.3.3, the sensitivity analysis can be integrated in the time integration scheme of the equations of motion. Consequently, the sensitivities are obtained as a supplementary result of the analysis with a low computation cost.

![Figure 3.6: Fully coupled method framework.](image)

### 3.3.2 Treatment of time-dependent constraints

The optimization problem (3.7) is stated in a continuous time domain. However, since numerical methods are used to solve the governing equations of the mechanical system, the functions involved in the optimization problem (3.7) are treated in a discrete time domain.
Let us consider a general function

$$f_j (q, \dot{q}, \ddot{q}, \lambda, p, t), \quad \forall t \in [t_i, t_f].$$  \hspace{1cm} \text{(3.9)}$$

After the time discretization, it becomes

$$f_j (q_n, \dot{q}_n, \ddot{q}_n, \lambda_n, p, t_n), \quad n = 1, \ldots, n_{\text{end}}$$ \hspace{1cm} \text{(3.10)}$$

where $n$ numbers the time steps. Since $n_{\text{end}}$ can be large, incorporating directly the discretized function (3.10) in the optimization can be costly. Firstly, the high number of constraints complexifies the task of the optimizer. Secondly, using gradient-based algorithms, the gradient computation of the responses is required at each time step. Therein, particular treatments of the time-dependent constraints are reviewed and proposed below to ease the optimization process.

**Pointwise constraints**

A pointwise constraint is a constraint that is defined at each integration time step. A first possibility is to incorporate directly this discretized function in the optimization. In this thesis, this treatment is referred to as a *local formulation*. However, several treatments can be applied to the pointwise constraint before incorporating it in the optimization problem (Fig. 3.7) and these are hereafter detailed:

*All the time steps combined with an active set strategy*

The time-dependent constraint can basically be treated by considering all the time steps. An active constraint set strategy can slightly reduce the number of constraints by neglecting the non-active time steps (Fig. 3.7(a)).

*All the local maxima*

A more radical treatment consists in considering all the local maxima of the response as constraints (Fig. 3.7(b)). Additional effort is required to track the local maxima. Grandhi et al. (1986) suggested an algorithm to find the maxima.

*All the local maxima and their neighborhood*

The previous treatment may suffer from convergence difficulties since the local maximum points can vary as the design proceeds. Indeed, a local maximum can move to a different time step at the next iterations. Including a couple of points around each maximum may help the convergence. The number of constraints is marginally increased while remaining relatively moderate (Fig. 3.7(c)).

*Worst case approach*

A simplistic treatment is to restrict the constraint to the worst case approach, i.e. the maximum violated response (Fig. 3.7(d)). As a consequence, a single constraint is considered except if multiple points have the same maximum value. However, this treatment generally exhibits a slow convergence or divergence as the worst case time step generally changes in a discontinuous way as the optimization proceeds. While this treatment seems to be very restrictive, it has been used in
several studies, e.g. Haug and Arora (1979) and Oral and Kemal Ider (1997).

Figure 3.7: Treatments of a pointwise constraint.
Chapter 3. Structural optimization of flexible components within a MBS approach

Functional constraints

In order to circumvent the difficulty of incorporating the \( n_{\text{end}} \) constraints related to Equation (3.10) in the optimization problem, the continuous form of this equation can be replaced by a single equivalent functional. The equivalent functional is expressed as

\[
F_j = \int_{t_i}^{t_f} \langle f_j (q, \dot{q}, \ddot{q}, \lambda, p, t) \rangle \, dt
\]

where

\[
\langle f_j (q, \dot{q}, \ddot{q}, \lambda, p, t) \rangle \equiv \begin{cases} 0 & \text{if } f_j < \bar{f}_j \\ f_j - \bar{f}_j & \text{if } f_j \geq \bar{f}_j \end{cases}
\]

It follows that satisfying \( F_j \leq 0 \) is equivalent to satisfying \( f_j \leq \bar{f}_j \). More details about this approach are given in Feng et al. (1977), Kocer and Arora (2002) and Kang et al. (2006).

The concept of using mathematical tools to transform many active or violated constraints, e.g. Equation (3.10), into one or a few constraints, is denoted as a global formulation in this thesis. Other mathematical tools can be used to perform this reduction.

Let us exemplify the use of the \( p \)-norm function in the particular case where the function \( f_j^+ \) has only positive values, i.e. \( f_j^+ \geq 0 \). Mathematically, the constraint reads

\[
\| f_j^+ (q, \dot{q}, \ddot{q}, \lambda, p, t) \|_p = \left( \int_{t_i}^{t_f} \left( f_j^+ \right)^p \, dt \right)^{1/p} \leq \| \bar{f}_j^+ \|_p
\]

where \( p \in \mathbb{R} \) and \( p \geq 1 \). If \( p = 2 \), one resorts to the Euclidean norm and dividing the integral by the time duration yields

\[
\sqrt{\frac{1}{t_f - t_i} \int_{t_i}^{t_f} \left( f_j^+ \right)^2 \, dt} \leq \| \bar{f}_j^+ \|_2
\]

which can be interpreted as the root mean square value of the constraint. When a global formulation is adopted to agglomerate the response function \( f_j^+ \), it should be noted that the constraint bound definition can become more difficult since it is no longer directly related to the physical response of the system but to the agglomerated response. If the parameter \( p \to \infty \), the \( p \)-norm reaches the infinity norm, also known as the maximum norm, i.e.

\[
\| f_j^+ (q, \dot{q}, \ddot{q}, \lambda, p, t) \|_\infty = \max_t \left( f_j^+ (t) \right).
\]

This formulation enables to identify the maximum value of the function, however, the infinity norm is a non-differentiable function. We note that the infinity norm leads to a similar formulation as the worst case approach.
Influence on the design space for MBS optimization

The design problem of MBS components is quite complex and poor convergence properties are encountered if the problem is not properly formulated. Indeed, the existence of significant couplings between vibrations and large amplitude motion, the influence of the changes of component inertial property on the vibrations as well as the interactions between flexible components lead to a daunting task for the optimizer. Article [1] in appendix is mainly concerned with the formulation of the optimization problem. Several treatments of time-dependent constraints have been investigated and discussed.

In order to tightly control the optimized design, it is required to consider one constraint at each time step. This local formulation can be coupled with an active set strategy. However, this formulation generally involves numerous constraints which hinder the optimization convergence. Moreover, it turns out that the design space resulting from such a formulation exhibits a lot of oscillations and is tortuous (Fig 3.8(a)). It follows that the design space is not the most suitable for gradient-based algorithms. Global formulations agglomerate the entire response into a few constraints and ease the convergence even if the resulting function is nonlinear since it involves a reduced number of constraints. Unfortunately, the precise control at each time step is lost due to their global nature. Nonetheless, global formulations create a smooth design space which is really convenient and well-suited for gradient-based algorithms (Fig 3.8(b)).

As an illustrative example, Figure 3.8 represents the design space of the mass minimization problem of a 2-dof robot subject to a trajectory tracking constraint. The robot has 6 design variables (arm thickness) and the design space is plotted when varying design parameters \( p_5 \) and \( p_6 \) while others are fixed. The smoothness characteristics previously explained can be observed. More details about the adopted formulation in this example are given in Article [1].

\[
\begin{align*}
\text{(a) } f_j(s, t_n) &\leq 10 \text{ mm}, \quad n = 20. \\
\text{(b) } \frac{1}{n_{\text{end}}} \sum_{n=1}^{n_{\text{end}}} f_j(s, t_n) &\leq 5 \text{ mm}.
\end{align*}
\]

Figure 3.8: Design space representation for a local formulation at time step \( n = 20 \) (a) and for a global formulation (b).
3.3.3 Sensitivity analysis of MBS

Sensitivity analysis is the essential link between the system analysis and the numerical optimization. The sensitivities indicate the influence of parameters over the system response but they are also needed to construct structural approximations of the original problem (Etman, 1997). Using the fully coupled method, the sensitivity analysis can be costly if not addressed with care as a dynamic response optimization is involved.

Several works have been carried out to develop an accurate and efficient design sensitivity methods for MBS. In the case of kinematic systems, Sohoni and Haug (1982) were amongst the first to propose a method generating the equations for both the primal analysis and the sensitivity analysis. The dynamics was included in the equations by Haug and Sohoni (1984). Later on, several authors contributed to the development of sensitivity analysis methods (for instance, Hsieh and Arora, 1984; Ashrafuon and Mani, 1990; Bestle and Seybold, 1992; Cardoso and Arora, 1992; Tortorelli, 1992; Wasfy and Noor, 1996; Dias and Pereira, 1997; Brüls and Eberhard, 2008; Ding et al., 2008; Dong et al., 2011).

Brüls and Eberhard (2008) proposed a semi-analytical direct differentiation technique to perform the sensitivity analysis for dynamic systems with large rotations. They established close connections between the structure of the sensitivity equations and of the linearized dynamic equations of motion. Therein, they proposed to use the algorithm developed for the original problem as well as for the sensitivities. Deriving the equations of motion and after some algebra (see e.g. Brüls and Eberhard, 2008), the sensitivity equations are stated as

\[
\begin{align*}
\mathbf{M} \frac{d\mathbf{q}}{dp_i} + \mathbf{C}_t \frac{d\mathbf{q}}{dp_i} + \mathbf{K}_t \frac{d\mathbf{q}}{dp_i} + k\Phi^T \frac{d\mathbf{\lambda}}{dp_i} &= -\frac{\partial \text{res}}{\partial p_i}, \\
k\Phi \frac{d\mathbf{q}}{dp_i} &= -k \frac{\partial \Phi}{\partial p_i}.
\end{align*}
\] (3.16)

It can be observed that their structure resembles the structure of the linearized dynamic equations of motion (2.20).

To evaluate the sensitivities \(d\mathbf{q}/dp_i, \frac{d\mathbf{q}}{dp_i}, \frac{d\mathbf{q}}{dp_i}\) and \(d\mathbf{\lambda}/dp_i\), all the terms of Equations (3.16) have to be computed. The pseudo-loads, \(\frac{\partial \text{res}}{\partial p_i}\) and \(\frac{\partial \Phi}{\partial p_i}\), are approximated using a finite difference method which requires \(n_v\) evaluations of the residual \(\text{res}|_{p+\Delta p_i}\) and \(\Phi|_{p+\Delta p_i}\) at each time step where the parameter perturbation is \(\Delta p_i = [0...0, \Delta p_i, 0...0]\). Also, the structural matrices \(\mathbf{M}, \mathbf{C}_t\) and \(\mathbf{K}_t\) must be evaluated. They cannot generally be retrieved from the primal analysis since they are aggregated in the tangent iteration matrix \(\mathbf{S}_t\), see Equation (2.24).

Ergo, a part of Article [2] is dedicated to an alternative sensitivity analysis formulation to ease the computational solution of Equation (3.16). A semi-analytical method is also considered to establish the sensitivity equations, derived from the residual form of
the equations of motion (2.11). After some developments detailed in Article [2], the sensitivity equations read

\[
- \mathbf{S}_t \begin{bmatrix} \frac{dq}{dp_i} \\ \frac{d\lambda}{dp_i} \end{bmatrix} = \begin{bmatrix} \frac{1}{\Delta p_i} \mathbf{res}_{pert} \\ \frac{k}{\Delta p_i} \Phi_{pert} \end{bmatrix}
\]

(3.17)

where

\[
\mathbf{res}_{pert} = \mathbf{res} \left( q_{|p}, \dot{q}_{|p} + \frac{dq}{dp_i} \bigg|_{p} \Delta p_i, \ddot{q}_{|p} + \frac{d\ddot{q}}{dp_i} \bigg|_{p} \Delta p_i, \lambda_{|p}, t, p + \Delta p_i \right), \quad (3.18)
\]

\[
\Phi_{pert} = \Phi \left( q_{|p}, p + \Delta p_i \right). \quad (3.19)
\]

The sensitivity equations (3.17) have several interesting properties. The tangent iteration matrix \( \mathbf{S}_t \) itself is involved in Equation (3.17), which has already been computed and factorized during the primal analysis. Hence, while many Newton iterations are required to evaluate the primal response \( \mathbf{q}_n \), only \( n_v \) back-solves are required to obtain its derivatives \( \frac{dq}{dp_i} \) if the convergence criterion of the Newton-Raphson iterative scheme is sufficiently small. Indeed, it is reasonable to use the tangent iteration matrix of the converged Newton-Raphson iteration (i.e. without recomputing it with the updated values \( \mathbf{q}_{n+1} \), etc.).

The perturbed terms, \( \mathbf{res}_{pert} \) and \( \Phi_{pert} \) can efficiently be computed. MBS simulation codes generally possess a function to compute the residuals. Therefore, the perturbed residuals in Equation (3.17) can be handily evaluated by calling this function with the perturbed arguments. Finally, the proposed sensitivity analysis method can easily be incorporated in the generalized-\( \alpha \) time integration scheme where the sensitivities are subsequently obtained as an additional result of the primal analysis.

3.4 Weakly coupled method

The weakly coupled method reformulates the optimization problem (3.7) such that the dynamic response of the system is replaced by a series of static responses, i.e. at each time step \( t_n \), the component deformation under the dynamic loading is mimicked by an equivalent static load (ESL). Hence, all the standard techniques of static response optimization can be applied to solve the reformulated problem. This section introduces the principles of the ESL method and the ESL evaluations adapted to different MBS formalisms. The formulation of an equivalent optimization problem and the framework of the optimization process are then described, concluding the section.
3.4.1 ESL evaluation

ESL for an isolated structure

Safety factors, dynamic amplification factors, designer’s experience, etc, were tradition-
ally used to convert a dynamic loading into static loads and to account for unmodel-
ed phenomena. However, this approach may increase the weight of the structure and de-
crease its reliability, i.e. the design is not optimal with respect to the actual loading
cases. The concept of converting a dynamic loading into static loads has been clarified
with the ESL method that was introduced for the structural optimization of an isolated
structure subjected to a dynamic loading (Choe et al., 1996; Choi and Park, 1999). The
authors proposed to define the ESL based on the displacement field resulting from the
dynamic loading as follows:

“When a dynamic load is applied to a structure, the equivalent static load is defined as
the static load that makes the same displacement field as that by the dynamic load at
an arbitrary time”.

Hence, the dynamic loading is mimicked by a series of static loads, namely the ESL, that
gives at each time step the same displacement field as the one given by the dynamic
loading. Regarding the analysis, this transformation is useless. However, the ESL
utility lies in the optimization procedure where they allow transforming the dynamic
response optimization into a static response optimization problem by regenerating the
displacement field from only static loads.

ESL combined with a floating frame of reference formulation

Kang et al. (2005) extended the previous definition to optimize components of flexible
MBS. To define the ESL, they considered that the component is isolated from the
system and that the displacement field is evaluated with respect to the body-attached
frame. They developed the method for MBS dynamics based on a floating frame of
reference formulation. As previously introduced, this thesis targets to extend the ESL
method to MBS dynamics based on a nonlinear finite element formalism. Indeed, the
latter formalism is appealing as its generality enables to analyze complex systems, and
its formulation is suitable to perform more advanced optimization processes such as
topology optimization.

The development of an ESL method for MBS optimization can be decomposed in
three steps. Firstly, a term, that can be identified as a force, must be extracted from
the equations of motion. It must be demonstrated that this force is able to generate
the same displacement as the displacement field resulting from the dynamic loading
at a given time step in a body-attached frame. Secondly, the method relies on the
optimization of isolated components, i.e. they have been decoupled from the system.
As a consequence, boundary conditions must be enforced to prevent rigid body modes in
the static analysis. Thirdly, if the small deformation assumption is valid, a linearized
problem must be derived from the nonlinear equations governing the motion of the system.

These three steps are naturally fulfilled when adopting the floating frame of reference formulation mainly as this formalism treats separately the rigid body motions and elastic deformations. Indeed, by isolating the last row of the equations of motion (2.1) related to the elastic coordinates, it is straightforward to identify the ESL that, for body $b$, reads

$$K^b_{ff}q^b_f = g^b_{eq} = -m^b f\ddot{x}_0^b - m^b f\dot{\theta}_0^b - m^b f\ddot{q}_f^b - C^T_{q^f} \lambda + \left( g^b_{ext} \right)_f + \left( g^b_{vel} \right)_f .$$

Moreover, the problem of the boundary conditions is handily circumvented since the floating frame of reference formalism already includes boundary conditions to connect the floating frame to the moving body. For instance, Shabana (2013) employs the Component Mode Synthesis method to introduce flexibility with this formalism, wherein boundary conditions are applied for the modal analysis. Hence, identical boundary conditions are adopted to fix all rigid body modes during the static analysis. Finally, the linearization of the original problem is not necessary since linear elasticity assumption is usual, so that Equation (3.20) is linear.

The extension to nonlinear finite element formalisms is not straightforward. Articles [3]-[4] in appendix are concerned with the ESL evaluation for a classical nonlinear finite element formalism and a Lie group formalism, respectively.

**ESL combined with a classical nonlinear finite element formalism**

In contrast to the floating frame of reference formulation, the equations of motion using a classical nonlinear finite element formalism (Géradin and Cardona, 2001) are developed in an inertial frame, i.e. the elastic forces are not expressed in a body-attached frame. Moreover, rigid body motions and elastic deformations exhibit no decoupling, in addition to the fact that the tangent stiffness matrix is not constant and evolves with the system configuration. As a result, the ESL evaluation becomes a more arduous task.

The evaluation of ESL is not as easy as isolating a term directly from the equations of motion as in Equation (3.20). The proposed method evaluates the ESL in a post-processing step of the MBS analysis, without modifying the analysis. The approach relies on the definition of a corotational frame that allows establishing the transformation laws to switch from a current configuration to a reference configuration. Hence, a single tangent stiffness matrix for the reference configuration $K_f^b(t_{ref})$ is considered instead of a different tangent stiffness matrix for each time step, since the latter evolves with the system configuration. The ESL are subsequently evaluated in the corotational frame thanks to a local generalized displacement vector $u^b_n$ that measures the deflection with respect to the undeformed configuration (Fig. 3.9). During the static analysis, rigid body modes are prevented using the boundary conditions associated
with the definition of the corotational frame. Also, the linearization is not necessary as nonlinearities are filtered out by the use of the corotational frame. It follows that the ESL in the corotational frame for the component $b$ at time step $t_n$ reads

$$ \mathbf{g}_{n,eq}^b = \mathbf{K}_t^b(t_{ref}) \mathbf{u}_n^b. $$  \hfill (3.21)

Figure 3.9: Description of the deflection of node $i$ in body $b$ with respect to a corotational frame.

**ESL combined with a Lie group formalism**

While still describing the MBS dynamics via a nonlinear finite element formalism, the Special Euclidean group $SE(3)$ exhibits several attractive properties for the weakly coupled approach. In particular, combining the Special Euclidean group $SE(3)$ with the left invariant representation of derivatives leads to a tangent stiffness matrix $\mathbf{K}_t$ that can be considered as constant under the assumption of small deformations, i.e. the tangent stiffness matrix is independent of the system configuration.

Another interesting characteristic of this formalism is that the equations of motion are expressed in the nodal local frame of each node. This aspect is decisive to evaluate efficiently the ESL since it leads to the definition of the ESL vector for body $b$ merely as the internal force vector acting on this body. Article [4] demonstrates that applying the internal force vector $\mathbf{g}_{n, int}^b$ to the isolated body gives the same statically deformed configuration $\mathbf{H}_{n, stat}^b$ as the dynamically deformed configuration $\mathbf{H}_{n}^b$ up to a rigid body motion $\mathbf{H}_{rig}^b$, i.e. $\mathbf{H}_{n}^b = \mathbf{H}_{rig}^b \mathbf{H}_{stat}^b$. This non-uniqueness issue is fixed by enforcing some boundary conditions to prevent rigid body motions, which are denoted by the symbol $(\bullet)^\circ$. Figure 3.10 depicts the previous statements.

This formalism can naturally account for large deformations at the sole price of solving the nonlinear problem

$$ \mathbf{g}_{n, eq}^{int, bo} = \mathbf{g}_{n, eq}^{bo}. $$  \hfill (3.22)

Nonetheless, as small deformations are usually encountered, it is appealing to derive
3.4 Weakly coupled method

Figure 3.10: ESL evaluation in a Lie group formalism.

an equivalent linear static problem by performing a linearization of Equation (3.22)
around the undeformed configuration, which produces

\[ K^b \Delta n_{stat}^b = g_{n,eq}^b. \]  

(3.23)

The term \( \Delta n_{stat}^b \) can be interpreted as a small increment vector that binds the statically
deformed configuration \( H_{stat}^b \) to the reference configuration \( H_{ref}^b \).

3.4.2 Formulation of the optimization problem

By definition, the weakly coupled method reformulates the original dynamic optimization
problem (3.7) such that the dynamic response of the system is replaced by a series
of equivalent static responses. Thusly, Kang et al. (2005) proposed to solve the following
static response optimization problem wherein ESL, denoted by \( g_{n,eq} \), are incorporated

\[
\begin{align*}
\text{minimize} & \quad f_0 (p) \\
\text{subject to} & \quad K^b (p) q_{n,eq}^b = g_{n,eq}^b, \quad b = 1, \ldots, n_b, \\
& \quad f_j (p, q_{n,eq}) \leq F_j, \quad j = 1, \ldots, n_c, \\
& \quad p_i \leq p_t \leq p_i, \quad i = 1, \ldots, n_v, 
\end{align*}
\]  

(3.24)

for \( n = 1, \ldots, n_{end} \) and where \( b \) numbers the components. In contrast to the optimization
problem (3.7), the equations of motion are replaced by a linearized version of the
equilibrium equation of each component for each time step. As a consequence, the op-
timization problem is solved using classical techniques of static structural optimization
with multiple load cases as presented in Section 2.2.

It is worth noticing that the formulation of the optimization problem includes all com-
ponents independently. Indeed, the weakly coupled method considers the optimization
of isolated components wherein the loading stems from the system analysis. Therein, the formulation of multicomponent-based constraints, i.e. design constraints involving several components, cannot be treated. For instance, such a constraint can be used to restrict the global behavior of the system. Exceptions exist when the multicomponent-based constraint can be transformed into several component-based constraints. Article [3] discusses the equivalence between the optimization problem formulations resulting from the weakly and fully coupled methods. It is shown that both methods can converge towards the same optimized design when the optimization problem can be formulated in an identical manner.

### 3.4.3 Framework of the optimization process

The framework of the optimization process for the weakly coupled method, illustrated in Figure 3.11, differs from the fully coupled method framework depicted in Figure 3.6. Indeed, the MBS analysis and the optimization process are no longer fully coupled but coupled via an intermediate step related to the ESL process.

The optimization problem formulation (3.24) considers that each component $b$ is loaded by as many load cases as the number of time steps. However, the ESL are fixed during the static response optimization process. Hence, to account for the effects of design modifications over the ESL, cycles are needed between the MBS analysis and the static response optimization. To solve the design problem using the weakly coupled method, Choi and Park (2002) proposed an algorithm to loop between the MBS analysis and the optimization process, which proceeds, apart from the stopping criteria, as follows:

1. Initialize the design variables and set the cycle counter to $it = 0$.
2. Perform a flexible MBS analysis.
3. Process the ESL.
4. If $it = 0$, go to step 5. If $it > 0$ and if

$$\frac{\sum_{n=1}^{t_{end}} \| g_{n,eq,it}^b - g_{n,eq,it-1}^b \|}{\sum_{n=1}^{t_{end}} \| g_{n,eq,it-1}^b \|} < \varepsilon,$$

then, stop. Otherwise go to step 5.
5. Solve the static response optimization problem (3.24). The iterations to solve this optimization problem are denoted as inner iterations.
6. Set $it = it + 1$ and go to step 2.

Figure 3.11 illustrates the algorithm. Stolpe (2014) discussed the convergence of the solution obtained using the weakly coupled method towards the optimal solution of the original dynamic response optimization problem. Moreover, the author criticized the proof establishing that if the ESL algorithm terminates then the KKT conditions of the original problem and the final sub-problem are identical (Park and Kang, 2003). Stolpe (2014) suggested a modified version for which the requested result is proven.
3.5 Weakly vs Fully coupled method

The choice of an optimization approach to perform the structural optimization of MBS components strongly depends on the considered application.

If the optimization problem incorporates multicomponent-based constraints, i.e. not limited to the response of a lone component, and that these constraints cannot be properly translated into component-based constraints, the fully coupled method is required. When the optimization problem formulation enables to use both methods, our experience shows that they can converge towards the same optimum.

The weakly coupled method generally lessens the CPU time as it avoids the expensive computation of the sensitivities. Mechanical systems with a rather moderate flexibility generally require less dynamic analyses to converge when employing the weakly coupled approach. However, this reduction is partly counterbalanced by inner iterations performed by the static response optimization at each cycle albeit these are based on static computations.

The fully coupled method is completely general and accommodates any types of constraints at the price of a more complex optimization process. For highly flexible systems, the fully coupled method may experience a faster convergence than the weakly coupled method since the ESL can drastically change from one cycle to another, hardening the
convergence. However, the designer must have a strong knowledge of the mechanical system dynamics to properly formulate the optimization problem. An inappropriate formulation results in poor convergence properties.
Chapter 4

Summary of the work

This chapter briefly introduces the four articles given in the appendices, afterwards the contributions and impact of the thesis are detailed. The first two articles are related to the fully coupled method and the last two articles to the weakly coupled method. The first article mainly focuses on the time-dependent constraint formulation. The second one introduces the level set description of the component geometry and revisits the sensitivity analysis of MBS. The third article investigates the ESL evaluation adapted to a classical nonlinear finite element formalism to describe the MBS dynamics. Also, a comparison with the fully coupled method is performed. The last article is dedicated to the ESL evaluation by taking advantage of the attractive properties of the Lie group formalism.

4.1 Summary of the articles

4.1.1 Formulation of time-dependent constraints for MBS optimization, Article [1] (Appendix A)

Article [1] is concerned with the fully coupled method which enhances most existing studies that are limited to weakly coupled (quasi-) static or frequency domain loading conditions. The difficult treatment of time-dependent constraints is investigated as it turns out to be a central point to establish a robust and reliable method. Indeed, the resulting dynamic response optimization problem is challenging to solve and naive implementations may lead to inaccurate and unstable results. The efficiency of the different formulations are explained by analyzing the complex nature of the design space. Also, the influence of the optimization algorithms on the convergence is analyzed. The introduced concepts and discussions are illustrated on two numerical applications: the mass minimization of a 2-dof robot subject to a trajectory tracking constraint and the optimization of a slider-crank mechanism.
4.1.2 Level set techniques and sensitivity analysis, Article [2] (Appendix B)

Article [2] is also dedicated to the fully coupled optimization method for the structural optimization of MBS components. Although, the component geometry is implicitly defined by a level set description leading to a generalized shape optimization problem. The optimization problem is solved via efficient gradient-based optimization methods requiring the gradients of cost and constraint functions. Hence, the sensitivity analysis is deeply revisited and reformulated to facilitate its implementation and retain its computational efficiency. The procedure is illustrated with the optimization of a 2-dof robot and a slider-crank mechanism.

4.1.3 Weakly coupled method in a classical nonlinear finite element formalism and comparison with the fully coupled method, Article [3] (Appendix C)

Article [3] deals with the weakly coupled method and is composed of two major parts. The first part of the work concerns the ESL evaluation that strongly depends on the adopted formulation to describe the MBS dynamics. Initially, the ESL evaluation has been developed based on a floating frame of reference formulation. Here, the standard ESL evaluation is extended to a nonlinear finite element formalism. The latter formalism is totally general to analyze complex MBS and is convenient to perform advanced optimization problems such as topology optimization. An original procedure is proposed to evaluate the ESL in a post-processing step. The second part focuses on a detailed comparison between the fully and the weakly coupled method. Our position is supported by several numerical examples. At the light of the comparison results, it is concluded that the fully coupled method is more general and accommodates any types of constraints at the price of a more complex optimization process.

4.1.4 Weakly coupled method in a Lie group formalism, Article [4] (Appendix D)

Article [4] continues along the ESL evaluation based on a nonlinear finite element approach. As previously mentioned, this approach is appealing due to its generality to analyze mechanisms and its convenience to perform advanced optimization problems such as topology optimization. In this paper, the nonlinear finite element approach relies on a Lie group formalism exhibiting attractive properties to evaluate the ESL. In particular, the selected Lie group formalism expresses the equations of motion in the local frame. An original method to efficiently evaluate the ESL is proposed by taking advantage of these interesting properties. Several standard examples validate the method.
4.2 Contributions and impact

The work presented in this thesis focuses on the coupling between structural optimization techniques and multibody system simulation tools to perform an integrated optimization of flexible components. While most of the structural optimization developments have been conducted under (quasi-)static loadings or vibration design criteria, the proposed approach aims at considering as precisely as possible the effects of dynamic loading in mechanical systems under service conditions. Two main coupling methods between the MBS analysis and the numerical optimization have been identified: the weakly and the fully coupled methods.

The weakly coupled method has been used for years and is nowadays implemented in commercial software tools. However, this approach was limited to floating frame of reference or rigid body MBS formalisms. This thesis extends the weakly coupled method to a nonlinear finite element approach, which is not straightforward since the formalisms rely on different fundamental concepts. The nonlinear finite element approach is attractive as it is totally general to analyze complex mechanical systems and is well-suited for advanced optimization problems such as topology optimization. Two existing nonlinear finite element formalisms have been considered. A first method has been proposed to evaluate the ESL based on a classical nonlinear finite element method (Géradin and Cardona, 2001) in a post-processing step (Article [3]). A second method has been developed based on a Lie group formalism (Sonneville and Brüls, 2014) whose particular properties enable to efficiently evaluate the ESL (Article [4]).

In order to conduct a fair comparison between the optimization methods, it is important to consider the same MBS formalism to avoid discrepancies from the analysis part. Therein, we compared both weakly and fully coupled optimization methods based on a standard nonlinear finite element formulation. It is shown that both methods can converge toward the same optimum when the optimization problem can be formulated in a similar way (Article [3]). It is worth mentioning that the weakly coupled method considers the optimization of isolated components while the loading stems from the system analysis. Hence, the formulation of design constraints involving multi-components may be incompatible with the weakly coupled method. The fully coupled method is more general and accommodates any types of constraints at the price of a more complex optimization process.

The fully coupled method is a more challenging method as it relies on the time response coming directly from the MBS analysis. Studies on the treatment of time-dependent constraints have been initiated with the master thesis of Emonds-Alt (2010). In the present thesis, we pushed further the investigations (Article [1]). It results that a universal formulation, suitable for all problems, is difficult to find. To ensure convergence and efficiency, the formulation should rather be tailored to the considered application. However, guidelines about the formulation are proposed. Also, the sensitivity analysis has been deeply revisited and reformulated to facilitate its implementation and retain
its efficiency (Article [2]). Indeed, gradient-based optimizations are conveniently used since they require less iterations to converge than heuristic methods. Besides, the time computation of MBS analyses is more expensive than for static analyses.

Since MBS analyses are in essence highly nonlinear, it is attractive to develop an optimization problem parameterization that enables deep modifications of the geometry while keeping a simple optimization process. To achieve this, an original coupling between an implicit description of the geometry based on the level set method and a geometry mapping based on a volume fraction has been proposed (Article [2]). This coupling leads to a generalized shape optimization method wherein the component topology can change in a limited manner.

The weakly and fully coupled methods were first implemented and validated using mainly academical tools. The MBS analysis was performed using simulation tools developed at the University of Liège, the optimization process was conducted by scripts in Matlab (The MathWorks, Inc., 2012b) and the optimization algorithm was either MMA (Svanberg, 1987) or the algorithms of the Matlab optimization toolbox (The MathWorks, Inc., 2012a). Afterwards, the fully coupled method was implemented using commercial software tools. The MBS simulation was performed using Samcef Mecano¹ and the optimization process was conducted using the optimization shell Boss Quattro². The latter implementation was possible since the fully coupled method does not require modifications in the MBS simulation code in contrast to the weakly coupled method, if the sensitivity analysis is based on a finite difference scheme or already available.

The developments of this thesis were mainly realized in the framework of a research project, namely the LightCar project. This project facilitated establishing contacts with industrial partners interested to collaborate and validate the developments carried out in the thesis. In particular, the fully and weakly coupled methods were applied to optimize power-train components in collaboration with Toyota Motor Corporation and Jtekt Torsen companies.

Chapter 5

Conclusion and perspectives

5.1 Concluding remarks

This thesis focuses on the structural optimization of flexible mechanical system components. In contrast to the mechanism synthesis defining the mechanism at a system level in a conceptual phase, the detailed design of the mechanical components is addressed here. However, to design innovative and lightweight mechanical systems, the influence of the entire system should be accounted for, since the interactions between components strongly affect the optimal design. As a consequence, a system-based optimization approach incorporating a MBS simulation is adopted.

Throughout the thesis, a nonlinear finite element approach is chosen to describe the MBS dynamics for several reasons. First, the nonlinear finite element formalism accounts for both large rigid-body motions and elastic deflections of the structural components in an integrated way. It follows that the approach is totally general to analyze the deformations of complex mechanisms undergoing arbitrary joint motions. Moreover, the approach is suitable to perform advanced optimization problems such as topology optimization since the continuum domain is discretized into finite elements.

The adopted system-based optimization approach is completely general to perform the structural optimization of mechanical system components. In particular, the thesis firstly focuses on sizing and shape optimizations accounting for time-dependent constraints. Secondly, a generalized shape optimization is performed in which the topology can change in a limited manner whereas the geometry is still precisely described by CAD entities.

The structural optimization of flexible components within a MBS approach is tackled by means of two general methods, so that a comparison of their respective merits and limitations can be performed. It is demonstrated that the nonlinear finite element approach can be successfully coupled with the two optimization methods, namely the
weakly and the fully coupled methods. Moreover, it is shown that some problems can be solved by both methods, leading to similar optimized designs. However, some optimization problems cannot be solved by the weakly coupled method which thus appears less general than the fully coupled method.

5.2 Future work

This work is a contribution to the structural optimization of flexible components in MBS and numerous perspectives can be foreseen. Hereafter, several directions for future work are detailed, in direct relationship with the present work.

A first perspective is to implement the discussed optimization methods into a commercial code. As a result, more complex examples could be handily treated since the computational time would be lessened. Also, examples of structural topology optimization problems, which are not included in this thesis, can be treated using the proposed system-based optimization framework.

This work focused on a nested approach to solve the fully coupled optimization problem. In this approach, most of the computational effort is invested to solve the equilibrium equations (Amir et al., 2010). Conversely, future work may address the SAND (Simultaneous ANalysis and Design) approach which does not solve the equilibrium equations apart from the optimization process but incorporates them into the optimization process. Consequently, the optimization problem size is largely increased. However, the matrices exhibit interesting properties such as sparsity that enable to obtain an efficient optimization process. Regarding the optimization problem of MBS components, its size is even larger since the integration formulae must be added to the equilibrium equation. Nonetheless, the SAND approach could be an interesting approach to solve a combined problem of structural optimization and optimal control. Optimal control can be performed using a SAND formulation that is named “Direct transcription method” in robotics (Bastos Jr. et al., 2013). In that reference, simple examples demonstrated the ability of the SAND formulation to solve MBS optimization problems. Ergo, an interesting perspective would be to investigate the coupled optimal control/component structural optimization problem.

The weakly coupled method considers the optimization of isolated components where the loading comes from the MBS analysis. The resulting approach is somehow restrictive because the optimization problem must be formulated with functions related to a single component and not to several components. Furthermore, the method depends on a subjective choice of boundary conditions to remove the singularity of the stiffness matrix at the component level. An interesting perspective would be to extend the weakly coupled method to consider the whole system in the static response optimization process and to get rid of the implicit assumption of the optimization of isolated components. The Lie group formalism seems to be particularly well-suited since the tangent stiffness matrix of the system slightly changes during the motion of the system.
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Appendix A

Article 1

Appendix B

Article 2

Appendix C

Article 3

Appendix D

Article 4
