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► To cite this version:

Petre Enciu, Laurent Gerbaud, Frédéric Wurtz. Automatic Differentiation Applied for Optimization of Dynamical Systems. COMPUMAG 09, 17th Conference on the Computation of Electromagnetic Fields, Nov 2009, Florianopolis, Brazil. pp.Pages 249-250. hal-00439629

HAL Id: hal-00439629 https://hal.science/hal-00439629

Submitted on 8 Dec 2009

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Automatic Differentiation Applied for Optimization of Dynamical Systems

Enciu Petre*, Gerbaud Laurent* and Wurtz Frédéric*

*Grenoble Electrical Engineering lab. (G2ELab), UMR5269, CNRS/UJF/INPG ENSE3, Domaine Universitaire, BP 46, F-38402 Saint Martin d'Hères Cedex, FRANCE Email: Petre.ENCIU@g2elab.grenoble-inp.fr

Abstract—Simulation is ubiquitous in many scientific areas. Applied for dynamic systems usually by employing differential equations, it gives the time evolution of system states. In order to solve such problems, numerical integration algorithms are often required. Automatic Differentiation (AD) is introduced as a powerful technique to compute derivatives of functions given in the form of computer programs in a high level programming language such as FORTRAN, C or C++. Such technique fits perfectly in combination with gradient based optimization algorithms, provided that the derivatives are valued with no truncation or cancellation error. This paper intends to use Automatic Differentiation employed for numerical integration schemes of dynamical systems simulating electromechanical actuators. Then, the resulting derivatives are used for sizing such devices by means of gradient based constrained optimization.

I. INTRODUCTION

Sizing by optimization is nowadays of major interest since it provides a fast and reliable way to achieve, with low manufacturing costs, desired performances for products lacking of optimality usually by means of minimizing a cost function. We are particularly interested by constrained gradient based optimization using Sequential Quadratic Programming (SQP) algorithms [1]. Such algorithms require accurately valued derivatives of the objective function. This may be the origin of serious problems provided that often such functions may result from complex numerical algorithms. We are particularly interested in this paper by those objective functions resulting from numerical integration of Initial Value Problems (IVPs) of Ordinary Differential Equations (ODEs) simulating the motion of an active body actuated by the electromagnetic force in the context of electromechanical actuators.

A good compromise in the optimization context is Automatic Differentiation (AD) that is a term applied for a technique able to compute derivatives of functions described by computer programs. That is, this paper only uses AD for sizing dynamical actuators by means of gradient based constrained optimization. In particular, AD will be applied using ADOL-C tool [2].

II. OPTIMIZATION PROBLEM

This paper considers the particular optimal problem of an IVP formulated as in (1) to (5):

$$minimize \ J(x_f, P) \tag{1}$$

$$\dot{x} = f(x, u(x, P)) \tag{2}$$

$$\dot{x} = f(x, u(x, t, P)) \tag{3}$$

$$x(0) = x_0 \tag{4}$$

$$x_i(t_f) = \tilde{x}_f, \quad \tilde{x}_f \in P \tag{5}$$

where $x \in \mathbb{R}^n$ denotes the state with its associated initial values x_0 . In the paper, two formulations of the state system are intentionally specified. The formulation in (2) represents an autonomous system, meaning that the time variable does not appear in the differential equation, while the formulation in (3) refers to a non-autonomous system. $P \in \mathbb{R}^p$ is the constraint design parameters set and u denotes the control. The objective function J depends on the reached final states and parameters. Equality (5) represents the simulation end criterion in Fig. 1, meaning that the simulation stops when a state x_i reaches a prescribed final state, $\tilde{x}_f \in \mathbb{R}$. This implies the existence of the final time or response time, t_f , depending implicitly on parameters. Note that \tilde{x}_f makes part of design parameters.

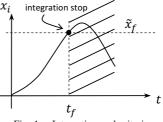


Fig. 1. Integration end criterion

The gradient based optimization algorithms applied for the optimization problem in (1) require the gradients of the objective function. These are evaluated like in (6) provided that the final states depend also on parameters:

$$\nabla J = \begin{bmatrix} \frac{\partial J}{\partial x_f} \end{bmatrix} \begin{bmatrix} \frac{\partial x_f}{\partial P} \end{bmatrix} + \begin{bmatrix} \frac{\partial J}{\partial P} \end{bmatrix}$$
(6)

Also, one may calculate the partial derivatives of the response time with respect to parameters set. So, the response time is carried out in optimization as a constrained parameter in addition to formulation in (1).

III. AUTOMATIC DIFFERENTIATION

Automatic Differentiation is introduced as a powerful technique that computes error-free derivatives, up to machine precision, of functions described as computer programs in high-level languages such FORTRAN or C/C++. In [5] a rich list of tools implementing AD is provided. Therefore, an AD tool could be a library that instruments a user program in order to be differentiated. Such tools require minor modifications on the initial source and they are implemented in packages like ADOL-C that is subject to this paper. In general they are using the operator overloading capabilities of certain programming languages such C++ and FORTRAN95. In order to value the partial derivatives in (1) one may employ ADOL-C over a numerical scheme integrating the ODE system in (2) or (3). The paper is then subject to two numerical integration strategies. First, it applies AD over an adaptive step size Rung-Kutta (RK) scheme as in (7):

$$x_{t_{i+1}}(P) = x_{t_i}(P) + h(P) \cdot \dot{\bar{x}}$$
(7)

where \dot{x} denotes a slope estimation and h is the integration step which depends on design parameters for an adaptive step size scheme.

Recent studies [4] were carried out for differentiating such schemes. The difference in [4] is that the response time is prescribed in advance at a fixed value. Our approach intends to make use of it as a constrained design parameter carried out further in optimization, so, its corresponding derivatives are to be valued as explained before.

Secondly, truncated Taylor Series (TS), as in [5] are applied to advance the solution of the ODE system in (2) or (3) over a time interval as in (8):

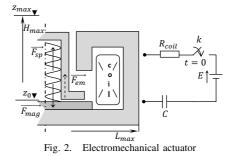
$$x_{t_{i+1}}(P) = x_{t_i} + \frac{x_1}{1!} \cdot h + \frac{x_2}{2!} \cdot h^2 + \dots + \frac{x_n}{n!} \cdot h^n \quad (8)$$

where $x_i = (d^i x)/(dt^i)$ denotes the i^{th} order Taylor coefficient. Paper [5] provides numerical solutions for adaptive step size schemes for ODE solvers using Taylor expansion. Interesting here is that AD is used for solving the dynamic system, provided that ADOL-C is capable to value high-order Taylor coefficients of the autonomous system in (2) supposing that f is sufficiently smooth. In the non-autonomous case like in (3) a special version of the ADOL-C routine responsible for Taylor coefficients valuation is applied. The differentiation of such integration schemes is made by using special drivers implemented in ADOL-C.

The differentiation of a RK integration scheme in (7) tends to be slower since the slope usually is represented by a complex algorithm in the case of schemes up to second degree. Contrary, the differentiation of (8) is faster since it represents a sum expansion. However, here a cost of high-order derivatives computation should be paid up to second degree. In the full paper comparisons will be carried out for both schemes in terms of efficiency as also as helpful aspects regarding the AD of such numerical integration algorithms.

IV. OPTIMIZATION GOAL

The benchmark in [6] of the electromechanical actuator modeling a circuit breaker in Fig. 2 is proposed for sizing by gradient constrained optimization. When the switch is turned off, the vacuum force produced by the magnet equilibrate the spring force. The simulation starts when the switch turns on. The electromagnetic force created by the coil cancels partially the magnet force. Consequently, the plunger will move, starting from initial position, z_0 , toward the upper bound, z_{max} .



The dynamical system of the proposed device combines both the equations of the electrical circuit feeding the coil and the movement equations. The states are:

$$\dot{x} = \left(\begin{array}{ccc} i & di/dt & z & v\end{array}\right) \tag{9}$$

The response time is found from the end criterion in (5), that is satisfied when the mobile plunger is bounded at z_{max} . A multi objective optimization problem raises form this particular case. These objectives are given in table I.

OPTIMIZATION SPECIFICATIONS		
Variable	Constraint	Formula
Percussion energy at z_{max}	[0.12, 10] J	$m \cdot v^2/2$
Response time	[0, 3.5] ms	-
Total force at z_{max}	15 N	-
Shock resistance at z_0	[2000 - 10000] m/s^{-2}	$\frac{F_{sp}-F_{mag}}{m}$
Total mass	minimize	-

TABLE I Optimization Specifications

The design parameters in (2) are represented by all geometrical parameters of the studied benchmark. The optimization results will be presented in the full paper.

V. CONCLUSION

This paper presents a particular optimization problem on a benchmark dealing with state variables in Ordinary Differential Equations. Runge-Kutta and Taylor expansion integration schemes are used to approximate these states. Both schemes are differentiated by employing Automatic Differentiation in order to value the gradients needed by SQP algorithms.

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