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A generic approach for the solution of nonlinear residual equations. Part III: Sensitivity computations

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ABSTRACT

Sensitivity analysis provides qualitative and quantitative information on the behaviour of the model under study, and offers an access to gradients that may be used for identification purposes. Such precious information may be obtained at a low development cost applying a generic automatic differentiation (AD) tool to the computer code implementing this model. Nonlinear residual problems solved through a path following method may be addressed too. In this paper, AD techniques are adapted to the Taylor-based asymptotic numerical method. A sensitivity study of a laminated glass beam to the perturbation of some material and geometric parameters, and the perturbation of elementary stiffness matrices illustrates the method.

1. Introduction

Within finite element formulations implemented in simulation codes, sensitivities [1,2] may be either (i) approximated by a finite difference scheme (FD), or computed through: (ii) the implementation of differentiated continuous equations, (iii) the implementation of differentiated discrete equations, or (iv) the differentiation of the code implementing the discrete equations, willingly performed using an automatic differentiation (AD) tool [3]. In a nutshell, AD views any computer code, even a large one, as a sequence of elementary operations and intrinsic functions, control and do-loop statements provided by the programming language. The AD is then performed applying the chain rule to this sequence, statement by statement, operation by operation. Using AD, computed derivatives are exact up to the machine precision. This generic technique constitutes a reliable solution for higher-order differentiation too, as demonstrated with the AD version [4] of the asymptotic numerical method (ANM) [5–7] for the solution of nonlinear problems through a continuation procedure. In the ANM, under analyticity assumptions, solutions are approximated as truncated Taylor series to be introduced in the discrete PDE problem of interest. This yields a sequence of linear problems involving the same matrix but different higher-order right-hand side terms. The differentiations stages are automated using the AD tool Diamant [8,9]. Sensitivities of ANM solutions were briefly presented in [10]. The present paper proposes a more thorough discussion on the subject to highlight the Diamant's capabilities in terms of sensitivity computations. A peculiar attention is brought to generality, ease of use and efficiency, as well as to the mechanical interest of such calculation.

These last decades, smart materials and adaptive structures have been extensively studied for a better knowledge and the improvement of their multifunctional properties. Sandwich structures including viscoelastic and/or piezoelectric layers are commonly used in industrial applications for noise and vibration control. Their modelling often results in nonlinear problems. Beside, sensitivity analysis tends to become a classical tool [11]. Applications are concerned with imperfection sensitivity [12], damage location [13] and vibration analysis [14,15]. Several approaches may be foreseen to compute sensitivities and to determine the parameters of larger influence. The choice of one method or the other usually depends on the complexity of the modelling equations, the availability of measurement devices and the number of parameters to study. For instance, sensitivities may be achieved through either laboratory experiments [16] or analytical approaches that can be successfully completed on rather simple systems of equations [14,17]. Most of the analytical studies, even based on a finite element formulation, assumes a manual differentiation to tackle peculiar problems [15,17]. Even Choi et al. [18,14] proposed a unified approach for design sensitivity analysis of nonlinear structural problems, this does not apply in a straightforward manner to the solution of nonlinear

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problems solved by asymptotic numerical method (ANM). In this paper, the AD tool Diamant is adapted to sensitivity computations. A sensitivity study of a laminated glass beam to the perturbation of some material and geometric parameters, and the perturbation of elementary stiffness matrices illustrates the method.

The outline of the paper is as follows. Theoretical aspects about AD, the Diamant version of the ANM and sensitivity analysis, are presented in Section 2. Implementation details are discussed in Section 3. Numerical experiments performed on a laminated glass beam are reported in Section 4. A summary and an outlook are provided to conclude.

2. Sensitivity computations with Diamant

Structural Mechanics modelling depends on some material and geometrical parameters p. In this regard, a crucial question that emerges immediately is this: what is the sensitivity of model's outputs to a given perturbation in the input parameters? This question can be answered at different levels of certainty by different approaches, from a qualitative manner obtained from experimental measurements of results stemming from successive trials, to quantitative methods based on the computation of first or second order derivatives. Within the last approach, great advances have been achieved with the development of AD [3]. Although this procedure has been applied with success in several scientific domains, it has been little applied in Structural Mechanics [1], and still less on nonlinear problems solved *via* a continuation technique.

This section first discusses AD basics for a better understanding of the diverse differentiation stages involved in the presented numerical process. Second, the ANM is turned into a generic AD-based method, namely the Diamant approach, for the solution of nonlinear continuation problems. A natural automation of sensitivity computations is then presented.

2.1. AD in a nutshell

Automatic differentiation (AD) is a set of techniques that enables to augment computer codes with derivative computation features. Within AD, any program execution ϕ is viewed as a composition of arithmetic operators and intrinsic functions. Its differentiation may be then automated using the chain rule and applying standard rules such as "the derivative of a sum is the sum of the derivatives", and so forth.

Higher-order differentiation is achieved through classical recurrence formulas. For instance, the multiplication $r = x * y$ is differentiated with respect to x and y applying the so-called Leibniz formula,

$$r_k = \sum_{j=0}^{k} x_j * y_{k-j}, \tag{1}$$

where, as defined in [3], x_k, y_k and r_k are Taylor coefficients at order k, *i.e.* scaled coefficients in the Taylor expansion of x, y and r respectively.

Two classes of AD tools exist. Given a computer code, source transformation tools like Tapenade [19] and ADiMat [20] are able to produce source codes containing derivative computation statements. These are mainly concerned with first order differentiation (in tangent linear mode and/or adjoint mode). Operator overloading tools like Adol-C [21], Rapsodia [22] and Diamant provide higher-order differentiation. The Taylor coefficient calculation is achieved by means of an operator overloading library as the vehicle of attaching derivative computations to the arithmetic operators and intrinsic functions provided by the programming language. The interested reader is referred to the automatic differentiation research community's web page http://www.autodiff.org for an exhaustive description of the available tools and usages.

2.2. The DIAMANT approach

The asymptotic numerical method (ANM) is a Taylor-based method devised for the solution of smooth nonlinear equilibrium systems of equations in general, and mechanical PDE problems in particular. Nonlinear problems we address are written in the generic residual form

$$\mathcal{R}(u(a,p),\lambda(a,p)) = 0, \tag{2}$$

where $\mathcal{R}(u(a,p),\lambda(a,p))$ and $u(a,p)$ are vectors of $\mathbb{R}^n$, and $\lambda(a,p)$ is a real-valued scalar parameter. For the sake of conciseness, the functional dependencies on modelling parameter p are hereafter omitted. The under-determined system (2) is usually closed adding the pseudo arc-length equation,

$$a = \left\langle u(a) - u(0), \frac{\partial u}{\partial a}(0) \right\rangle + (\lambda(a) - \lambda(0))\frac{\partial \lambda}{\partial a}(0), \tag{3}$$

where a is the path parameter.

Assuming $\mathcal{R}, u$ and λ to be analytical functions, the ANM approximates the solutions of (2) and (3) as Taylor expansions truncated at order K, that is

$$(u(a),\lambda(a)) = \left(\sum_{k=0}^{K} a^k u_k, \sum_{k=0}^{K} a^k \lambda_k\right), \tag{4}$$

where Taylor coefficients u_k and λ_k are, respectively, equal to $\frac{1}{k!}\frac{\partial^k u}{\partial a^k}(0)$ and $\frac{1}{k!}\frac{\partial^k \lambda}{\partial a^k}(0)$. Within the ANM, series (4) are introduced in the actual nonlinear problem. This yields a problem-dependent sequence of K linear systems involving the same tangent linear matrix, and higher-order differentiation recurrence formula to be written by hand [7]. For the sake of clarity the dependence in a is omitted in the following.

The Diamant approach [4] is the AD-based version of the ANM. As described in [8,9], Faá di Bruno generalized chain rule formula allows to split the Taylor coefficient $\mathcal{R}_k$ into three parts,

$$\mathcal{R}_k = \{\mathcal{R}_{1|u_1=Id,\lambda_1=0}\}u_k + \{\mathcal{R}_{1|u_1=0,\lambda_1=1}\}\lambda_k + \{\mathcal{R}_{k|u_k=0,\lambda_k=0}\} = 0, \tag{5}$$

where $\{\mathcal{R}_{1|u_1=Id,\lambda_1=0}\}$ is the tangent linear matrix of $\mathcal{R}$ differentiated with respect to u, $\{\mathcal{R}_{1|u_1=0,\lambda_1=1}\}$ is the tangent linear contribution of $\mathcal{R}$ differentiated with respect to λ, and $\{\mathcal{R}_{k|u_k=0,\lambda_k=0}\}$ represents higher-order contributions. In the latter, the use of null Taylor coefficients for u_k and λ_k cancels the tangent linear contributions already taken into account in the first two terms. Such generic decomposition allows for the automation of the ANM [8,9]:

- the Jacobian $\{\mathcal{R}_{1|u_1=Id,\lambda_1=0}\}$ is the same over the order. It may be constructed in an efficient way taking into account the finite element assembly mechanism [10],
- the higher-order term $\{\mathcal{R}_{k|u_k=0,\lambda_k=0}\}$ may be efficiently computed using a peculiar Diamant operator overloading library [8].

Consequently, the sequence of K generic linear systems related to the ANM and the path equation may be written

$$\begin{cases} \{\mathcal{R}_{1|u_1=Id,\lambda_1=0}\}u_k + \{\mathcal{R}_{1|u_1=0,\lambda_1=1}\}\lambda_k = -\{\mathcal{R}_{k|u_k=0,\lambda_k=0}\}, \\ a = (u_k - u_0)u_1 + (\lambda_k - \lambda_0)\lambda_1. \end{cases} \tag{6}$$

In practice, the calculation of $\{\mathcal{R}_{k|u_k=0,\lambda_k=0}\}$ and the solution of (6) are performed in an iterative manner from order 1 to order K.

2.3. Sensitivity computations

Linear systems (6) depend on modelling parameters p. In the ANM/Diamant context, sensitivities $\frac{\partial u_k}{\partial p}$ and $\frac{\partial \lambda_k}{\partial p}$ of Taylor coefficients