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A generic approach for the solution of nonlinear residual equations. Part I: The Diamant toolbox

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ABSTRACT

Sufficiently smooth nonlinear PDE problems may be addressed through the higher order derivative computations of the so-called Asymptotic Numerical Method (ANM). In this paper, we theoretically discuss the generic solution of nonlinear residual equations. We then propose a Matlab implementation of the ANM based on Automatic Differentiation which allows for significant improvements in genericity and ease of use. The Diamant toolbox we construct is applied to the study of the geometrical nonlinear behavior of a laminated glass beam. Numerical results and experimental performances demonstrate the efficiency of the Diamant tool.

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1. Introduction

Sufficiently smooth nonlinear PDE problems may be tackled through the higher order derivative computations of the so-called Asymptotic Numerical Method [1,2]. Truncated Taylor series are introduced in the PDE problem of interest to exhibit a sequence of linear systems following the same pattern. Each of these systems, one per order of differentiation, involves the tangent linear matrix and peculiar right-hand side terms containing higher order derivative formulae. It is worth noticing that these formulae differ from the classical differentiation recurrence formulae since they miss the term used in the construction of the tangent linear matrix. At given points, ANM computed series allow for cheap evaluations of approximate solutions in their vicinity. From a computational point of view, the ANM alternates higher order derivative calculations and linear system solutions in an iterative process. Due to this specific features, the ANM series computations were mainly handwritten. Some automation efforts were made [3,4] for nonlinear PDE problems written under the prescribed form

$$\mathscr{R}(v,\lambda) = L_0 + L(v) + Q(v,v) + \lambda F = 0, \qquad (1)$$

where $\mathscr{R}(v,\lambda) \in \mathbb{R}^n$ is the residual vector depending on the unknown vector $v \in \mathbb{R}^n$ and the load parameter $\lambda \in \mathbb{R}$. In [3,4], the decomposition into functions L_0 (constant), L (linear) and Q (quadratic) remains a user concern.

Automatic Differentiation [5] (AD) is a generic approach that allows for higher order differentiation. The AD-based Diamant approach (as a French acronym for *DIfférentiation Automatique de la Méthode Asymptotique Numérique Typée*) has been targeted [6] for hiding the ANM differentiation aspects to the user. Within Diamant, right-hand side series computations are achieved by propagating Taylor coefficients of the residual $\mathscr{R}$ [6,7]. As presented here, theoretical aspects may be discussed in a generic fashion whatever the residual equations, the discretization method and the behavior law are.

From a computational point of view, Diamant relies on Operator Overloading (OO) as the vehicle for attaching our higher order derivative computations to the arithmetic operators and intrinsic functions provided by the programming language. We focus our attention on object-oriented Matlab programming techniques for an efficient and generic implementation of the ANM. Equivalent Diamant packages were developed in Fortran 90 [6] and C++ [7]. Once the differentiation abilities of the OO library are validated, the Diamant toolbox may be used with confidence for the solution of any smooth residual equation.

Laminated glasses are sandwich structures combining two or more glass sheets with one or more interlayers of elastomeric polymer (polyvinyl butyral, PVB). These are widely used as architectural glazing in contemporary buildings or as windscreens in automotive industries. Geometrical effects as well as the difference between the glass properties and the PVB time and temperature dependent properties induce complex nonlinear behaviors. This mainly explains why most literature on laminated glass is based

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upon experimental studies. A review may be found in [8–10]. Some analytical and numerical studies were recently developed for predicting the nonlinear behavior of laminated glass beams and plates. On the one hand, Aşik [8,9] applies an iterative method based on a finite difference scheme for the study of the geometrical nonlinear behavior of laminated glass beams and plates. As discussed in [8,9], a solution is reached using a tuned under-relaxation parameter. On the other hand, an analytical model is developed in [10] for analysis of the linear static behavior of laminated glass beam set on visco-elastic supports. A linear free vibration analysis [10] is also studied by means of a finite element method implemented within Matlab. In the present paper, we illustrate the Diamant abilities (genericity and efficiency) with a numerical study of geometrical nonlinear effects on laminated glass structures. The Diamant toolbox we present offers the genericity of both a finite element discretization and the Diamant approach.

The layout of the paper is as follows: Section 2 presents the higher order ANM equations on generic nonlinear PDE problems and Section 3 discusses the Diamant approach we adopt to tackle the differentiation stages. The Diamant toolbox allowing for an easy implementation of the ANM is described in Section 4. Usage and performances are presented in Section 5 on a nonlinear laminated glass ODE problem. Some perspectives are proposed as a conclusion.

2. Setting of the generic problems

The generic nonlinear residual equation we consider is

$$\mathscr{R}(v,\lambda) = 0, \tag{2}$$

where $\mathscr{R}(v,\lambda) \in \mathbb{R}^n$ is the residual vector depending on the unknown vector $v \in \mathbb{R}^n$ and the load parameter $\lambda \in \mathbb{R}$. Solutions (v,λ) of this under-determined system of n nonlinear equations in $n+1$ unknowns form a branch that may be described considering v and λ as functions of a path parameter a. Hereafter we consider the pseudo-arc-length equation:

$$\text{Path eq.}: a = \left\langle v(a) - v(0), \frac{\partial v}{\partial a}(0) \right\rangle + (\lambda(a) - \lambda(0))\frac{\partial \lambda}{\partial a}(0), \tag{3}$$

where $\langle .,. \rangle$ is a dot product. When $\mathscr{R}$ is "quadratic" in v, *i.e.* $\mathscr{R}$ verifies Eq. (1), two "less" generic formulations may be written

$$\begin{aligned} &\text{Case A}: \mathscr{R}_A(v,\lambda) = A(v)S(v) + \lambda F = 0, \\ &\text{Case B}: \mathscr{R}_B(v,\lambda) = B(v)v + \lambda F = 0. \end{aligned} \tag{4}$$

In former equations, the matrix $A(v)$ depends linearly on v whereas the matrix $B(v)$ and the vector $S(v)$ depend on v in a nonlinear fashion. The load vector $F \in \mathbb{R}^n$ is a constant. The nonlinear laminated glass problem we consider in Section 5 agrees with both formulations.

In order to apply the ANM we assume that $a \mapsto v(a)$, $a \mapsto \lambda(a)$, $(v,\lambda) \mapsto \mathscr{R}(v,\lambda)$, $v \mapsto B(v)$ and $v \mapsto S(v)$ are analytic functions. Taylor coefficients at order k of $v(a)$, $\lambda(a)$, $b(a) = B \circ v(a)$ and $s(a) = S \circ v(a)$ evaluated at point $a = 0$ are respectively denoted by $v_k = \frac{1}{k!}\frac{\partial^k v}{\partial a^k}(0)$, $\lambda_k = \frac{1}{k!}\frac{\partial^k \lambda}{\partial a^k}(0)$, $b_k = \frac{1}{k!}\frac{\partial^k (B\circ v)}{\partial a^k}(0)$ and $s_k = \frac{1}{k!}\frac{\partial^k (S\circ v)}{\partial a^k}(0)$. Following the ANM methodology, truncated Taylor series $\sum_{k=0}^K a^k v_k$, $\sum_{k=0}^K a^k \lambda_k$, $\sum_{k=0}^K a^k b_k$ and $\sum_{k=0}^K a^k s_k$ are introduced in (3) and (4). This yields:

$$\begin{aligned} &\text{Case A}: A\left(\sum_{k=0}^K a^k v_k\right)\left(\sum_{k=0}^K a^k s_k\right) + \left(\sum_{k=0}^K a^k \lambda_k\right)F = 0, \\ &\text{Case B}: \left(\sum_{k=0}^K a^k b_k\right)\left(\sum_{k=0}^K a^k v_k\right) + \left(\sum_{k=0}^K a^k \lambda_k\right)F = 0, \\ &\text{Path eq.}: \left\langle \left(\sum_{k=0}^K a^k v_k\right) - v_0, v_1 \right\rangle + \left(\left(\sum_{k=0}^K a^k \lambda_k\right) - \lambda_0\right)\lambda_1 = a. \end{aligned} \tag{5}$$

The use of the Leibniz formula and the identification of terms in a^k yield recurrent sequences of K linear systems of equations:

$$\begin{aligned} &\text{Case A}: \sum_{l=0}^k A(v_{k-l})s_l + \lambda_k F = 0, \quad \forall k = 1,\ldots,K, \\ &\text{Case B}: \sum_{l=0}^k b_{k-l}v_l + \lambda_k F = 0, \\ &\text{Path eq.}: \langle v_1, v_k \rangle + \lambda_1 \lambda_k = \delta_{1k}. \end{aligned} \tag{6}$$

Series s_k or b_k are formulation dependent. As noticed in [2], numerical results of the ANM do not depend on the implementation of formulation (6A), formulation (6B) or their equivalent quadratic form. Before Diamant was developed [6], the implementation of either the quadratic form or the series s_k or b_k was an user task.

Once implemented, truncated Taylor expansions $\sum_{k=0}^K a^k v_k$ and $\sum_{k=0}^K a^k \lambda_k$ are approximations of $v(a)$ and $\lambda(a)$ in the vicinity of $a = 0$ that allow for branch computations in path following problems [11]. Many nonlinear mechanical equations agree with the residual form (2). Plasticity [12], contact [13], nonlinear constitutive laws [14] as well as nonlinear eigenvalue problems [15] and nonlinear forced vibration problems [16] were already addressed by means of the ANM. An exhaustive review may be found in [2].

As discussed in the following, Diamant enables the evaluation of ANM series through a propagation of Taylor coefficients. This propagation may be achieved in an automatic fashion whatever the specificities of the problem – formulations (6A) or (6B), discretization method, constitutive law are.

3. The Diamant approach

The governing idea of the Diamant approach is the introduction of genericity in the ANM computations.

3.1. Theoretical basis

Our theoretical developments are based on the generic Faá di Bruno formula for the higher order differentiation of compound functions. It is worth noticing that we use it for theoretical purposes only: the actual computational differentiation is performed by means of AD techniques (see Section 4).

The Faá di Bruno formula applied to $B \circ v$ yields:

$$b^{(k)} = (B \circ v)^{(k)} = \sum_{l=1}^k B^{(l)} \beta_{k,l}(v^{(1)},\ldots,v^{(k-l+1)}), \tag{7}$$

where variables $v^{(k)} = k! v_k$ and $B^{(k)} = k! B_k = \frac{\partial^k B}{\partial v^k}(v(0))$ are the derivatives at order k of v and B, respectively, and $\beta_{k,l}(v^{(1)},\ldots,v^{(k-l+1)})$ (for $l = 1,\ldots,k$) are Bell polynomials [17] satisfying:

$$\beta_{k,l}(v^{(1)},\ldots,v^{(k-l+1)}) = \sum \frac{k!}{i_1!\cdots i_{k-l+1}!}\left(\frac{v^{(1)}}{1!}\right)^{i_1}\cdots\left(\frac{v^{(k-l+1)}}{(k-l+1)!}\right)^{i_{k-l+1}}. \tag{8}$$

This sum is over all partitions of k into l non-negative parts such that $i_1 + i_2 + \cdots + i_{k-l+1} = l$ and $i_1 + 2i_2 + \cdots + (k-l+1)i_{k-l+1} = k$. Hereinafter, theoretical developments are performed for $n = 1$ for the sake of clarity in the differentiation notations. As proved in [7], Eq. (6A) may be written as

$$\text{Case A}: L_T^A v_k + \lambda_k F = R_k^A, \tag{9}$$

where L_T^A is the tangent linear matrix satisfying

$$L_T^A v = A(v)S_0 + A(v_0)S_1 v, \quad \forall v. \tag{10}$$

Right hand-side terms are

$$R_k^A = -\sum_{l=1}^{k-1} A(v_{k-l})s_l - A(v_0)\left(\sum_{l=2}^k \frac{l!}{k!} S_l \beta_{k,l}(v^{(1)},\ldots,v^{(k-l+1)})\right), \tag{11}$$

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