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On a path-following method for non-linear solid mechanics with applications to structural and cardiac mechanics subject to arbitrary loading scenarios

S. Skatulla[a,b,*], C. Sansour[c,1]

[a] Computational Continuum Mechanics Group, Department of Civil Engineering, University of Cape Town, Cape Town, South Africa
[b] Centre for Research in Computational and Applied Mechanics, University of Cape Town, Cape Town, South Africa
[c] Faculty of Engineering, The University of Nottingham, University Park, Nottingham NG7 2RD, United Kingdom

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ABSTRACT

In computational solid mechanics path-following methods have been proven useful when dealing with non-monotonously evolving loading magnitudes as encountered e.g. in instability or softening behaviour. The present work derives from a displacement-based method a cavity-volume-based path-following method and considers its application specifically to cardiac mechanics problems. Both methods are able to account for an arbitrary number of simultaneously acting loading conditions. When applied to the *Newton-Raphson* method, the corresponding loading increments are computed by means of volume increments or point-wise prescribed displacement increments, respectively. No additional variables are required and the physics of the problem at hands is not altered. Both methods are implemented in an in-house meshfree modelling software and successfully applied to non-linear elastic and inelastic problems in structural mechanics. The cavity-volume control method, in particular, is demonstrated to accurately predict the highly non-linear elastic and anisotropic material behaviour encountered when modelling the heart. Albeit, the proposed methods can be equally used e.g. in finite element methods, they are very well suited for meshfree methods where the Kronecker delta property does not apply.

1. Introduction

Over the last four decades, computational solid mechanics has become widely accepted for the analysis of linear and non-linear structural problems of arbitrary geometry, loading and support conditions, material behaviour etc. In the non-linear case, the response of the structure can be complex and the load-displacement curve can be neither convex nor monotonic in one or both variables, the load and the displacements. Especially, in the presence of limit points in the load-displacement curves such as in stability analysis or softening behaviour of structures (damage, plasticity), the load increment cannot be formulated directly. Instead, the loading parameter itself is considered as an unknown which is solved via a constraint of some kind leading to so-called path-following methods. Early on, so-called arc-length methods have been developed to trace the load-displacement curves beyond limit points. Essentially, a side condition is formulated which links the increment of the load vector to an increment in the displacement vector. Starting from the original ideas of Riks (1972); 1979), where an orthogonality condition has been formulated as a side condition, many modifications have been proposed (Crisfield, 1981; Garcea et al., 2002; Ramm, 1981; Riks et al., 1996). Specifically for one-dimensional instability and bifurcation analysis, Eriksson (1998) introduced a generalised framework which is able to predict the structural behaviour for one or more governing parameters, e.g. loading magnitude, geometry etc. Geers (1999) proposed a unified framework for subplane methods featuring a self-adaptive solution control scheme for initial load estimation, adaptation and correction as well as sign prediction when passing limit points. In the context of ductile and brittle failure, dissipation-based approaches have been introduced by Lorentz and Badel (2004); Verhoosel et al. (2009), amongst others.

These methods have in common that the load increment is formulated as a, in general, non-linear function of the norm of the displacement vector. The function differs from one method to another and some would be more suitable to certain types of behaviour than others. Whatever the method, the load increments are in generally small and the calculation of the same could be cumbersome and time consuming. Alternatively, established in

* Corresponding author. Tel.: +27 21 6502595; fax: +27 21 6501455.
E-mail addresses: sebastian.skatulla@uct.ac.za (S. Skatulla), carlo.sansour@nottingham.ac.uk (C. Sansour).
[1] Tel.:+44 115 9513874; Fax:+44 115 9513898

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commercial software is the case of displacement control, where not the load vector but a displacement vector is prescribed driving the simulation. By multiplication with the stiffness matrix a corresponding load vector is generated. In this form, however, the method does not consider arbitrary load conditions. Moreover, these methods are formulated mainly for the finite element method where the Kronecker delta property applies. In contrast, many meshfree methods have no nodal degrees of freedom and the displacement-control must be defined differently.

In the present work, two straightforward but very efficient path-following methods are presented. They are characterized by the property that, on the one hand, the loading vector can be arbitrary but on the other hand, the loading increment is controlled by a choice of either volume or displacement increments rendering the methods volume or displacement-controlled ones, respectively. More in detail, the methods have the following features: 1) They are extremely simple and can be directly implemented; 2) In comparison with other available methods, it allows for large load increments; 3) The choice of the volume or displacement evolution which controls the calculation can be arbitrary as long as it is being physically meaningful; 4) As numerical experience shows, the methods are robust and, although they do not cover all cases, they can be efficiently applied to a large number of them; 5) The methods are formulated for multiple loading conditions that can exhibit each different monotonously as well as non-monotonously evolving loading magnitudes, as it is the case for the blood filling pressures in the heart chambers during the cardiac cycle.

The path-following method is implemented in the in-house modelling software SESKA. SESKA is a numerical modelling software based on the element free Galerkin method (EFGM) which uses moving least squares approximations (MLS) of the solution over the domain. For further details on EFGM and MLS methods, the reader is directed to the paper by Belytschko et al. (1994). It should be stressed again that the numerical methods outlined in the following can be applied to a finite element framework just as well.

The plan of this paper is as follows: Section 2 outlines the standard approach to solve a quasi-static non-linear solid mechanics problem. Subsequently, in Section 3 the displacement-control approach is introduced which is subsequently extended to a cavity volume-control approach in Section 4. In Section 5 various applications involving elastic and inelastic material behaviour successfully demonstrate the flexibility of both methods. The cavity-volume control method, in particular, is shown to accurately predict the highly non-linear elastic and anisotropic material behaviour of cardiac mechanics problems.

2. The variational principle and its linearization

Let us first consider a non-linear boundary value problem in the domain $\mathcal{B}$ with the boundary $\partial\mathcal{B}$. Dirichlet boundary conditions are prescribed on $\partial\mathcal{B}_D \subset \partial\mathcal{B}$ and Neumann boundary conditions are prescribed on $\partial\mathcal{B}_N = \partial\mathcal{B} \setminus \partial\mathcal{B}_D$.

Let $\mathcal{W}_{(ext)}$ define the external virtual work in the Lagrangian form as follows

$$\mathcal{W}_{(ext)} = \int_{\mathcal{B}} \mathbf{b} \cdot \delta\mathbf{u} \; dV + \int_{\partial\mathcal{B}_N} \hat{\mathbf{t}}^{(\mathbf{n})} \cdot \delta\mathbf{u} \; dA \,, \tag{1}$$

where $\delta\mathbf{u}$ denotes the virtual displacement vector, $\mathbf{b}$ the body force and $\hat{\mathbf{t}}^{(\mathbf{n})}$ the external traction vector prescribed on $\mathcal{B}_N$. dV is a volume element of domain $\mathcal{B}$, whereas dA is a surface element of its corresponding boundary $\partial\mathcal{B}$ with the outward surface normal vector $\mathbf{n}$.

Now let $\mathbf{F}(\mathbf{u}) = \mathbf{1} + \text{Grad}\,\mathbf{u}$ be the deformation gradient and define $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ as the right *Cauchy-Green* deformation tensor and $\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{1})$ as the *Green* strain tensor. To account for possible inelastic material response we consider the multiplicative decomposition of $\mathbf{F}$ into an elastic and an inelastic part $\mathbf{F} = \mathbf{F}_e\,\mathbf{F}_p$ and define $\mathbf{C}_e = \mathbf{F}_e^T\mathbf{F}_e = \mathbf{F}_p^{-T}\mathbf{C}\mathbf{F}_p^{-1}$ as the elastic right *Cauchy-Green* deformation tensor. We assume a general material response with an elastic range and let $\psi(\mathbf{C}_e(\mathbf{E}, \mathbf{F}_p))$ define the strain stored energy function per unit un-deformed volume. This definition can be modified as necessary. It is general enough for our considerations here. Then the variation of the internal potential with respect to $\mathbf{E}$ in the Lagrangian form reads as follows

$$\Psi_{(int)} = \int_{\mathcal{B}} \frac{\partial\psi}{\partial\mathbf{E}} : \delta\mathbf{E} \; dV \,. \tag{2}$$

Considering only mechanical processes, the first law of thermodynamics provides the following variational statement

$$\mathcal{F} = \Psi_{(int)} - \mathcal{W}_{(ext)} = \\ = \int_{\mathcal{B}} \mathbf{S} : \delta\mathbf{E} \; dV - \int_{\mathcal{B}} \mathbf{b} \cdot \delta\mathbf{u} \; dV - \int_{\partial\mathcal{B}_N} \hat{\mathbf{t}}^{(\mathbf{n})} \cdot \delta\mathbf{u} \; dA = 0 \,, \tag{3}$$

where Eqs. (1) and (2) have been substituted and $\mathbf{S}$ denotes the second *Piola-Kirchhoff* stress tensor given by

$$\mathbf{S} = \frac{\partial\psi}{\partial\mathbf{E}} \,. \tag{4}$$

The double dot operator (:) denotes the scalar product of tensors. This variational principle is supplemented by essential boundary conditions, the so-called Dirichlet boundary conditions

$$\mathbf{u} = \hat{\mathbf{u}} \quad \text{on } \partial\mathcal{B}_D. \tag{5}$$

In the case of inelastic deformations, the constitutive relations are to be extended to encompass evolution equations of the inelastic deformation itself, together with possible internal parameters. For details of these formulations the reader is referred to the standard text books (e.g. Bonet and Wood, 1997; Dunne and Petrinic, 2005; Simo and Hughes, 2006; Zienkiewicz and Taylor, 2005). Specifically, for the one used in the examples presented in this paper in Section 5, details can be found in Sansour and Kollmann (1998).

Now, considering the general case of finite strain and non-linear material behaviour, the above variational statement is solved incrementally and iteratively employing the *Newton-Raphson* method. For this, at each iteration step, i, of an incremental loading or time step, n, Eq. (3) is linearized using a first-order Taylor expansion in the vicinity of some known solution of the displacement field, i.e. solution $\mathbf{u}_n^{i-1}$ as obtained in the previous iteration step or for $i = 0$ the converged solution of the previous loading step, $\mathbf{u}_{n-1}$, which yields

$$\mathcal{F}\left(\mathbf{u}_n^i\right) = \mathcal{F}\left(\mathbf{u}_n^{i-1} + \Delta\mathbf{u}\right) = \mathcal{F}\left(\mathbf{u}_n^{i-1}\right) + \frac{\partial\mathcal{F}}{\partial\mathbf{u}}\Big|_{\mathbf{u}_n^{i-1}} \Delta\mathbf{u} \approx 0 \,, \tag{6}$$

where $\Delta\mathbf{u}$ is the incremental displacement field such that the unknown displacement field in the current iteration step $\mathbf{u}_n^i = \mathbf{u}_n^{i-1} + \Delta\mathbf{u}$. Making use of a numerical approximation of the displacement field, here MLS-approximations, the linearized problem formulation (Eq. (6)) results in a discrete equation system of the following form

$$[\mathbf{K}]_n^i[\Delta\mathbf{u}]_n^i = \left[\mathbf{f}_{(ext)}\right]_n^i - \left[\mathbf{f}_{(int)}\right]_n^i = [\mathbf{r}]_n^i \,, \tag{7}$$

where the external force vector $[\mathbf{f}_{(ext)}]_n^i$ corresponds to Eq. (1), the internal force vector $[\mathbf{f}_{(int)}]_n^i$ to Eq. (2), $[\mathbf{K}]_n^i$ denotes the tangent matrix and $[\mathbf{r}]_n^i$ the residual vector of the discrete equation system. As for the variational principle, we understand the tangent or stiffness matrix as a general one, which could be an elastic-plastic one, derived via a suitable integration method. Here too, the reader is referred to standard textbooks.

As mentioned before, the non-linear nature of the problem necessitates that the external loads $P \in \{\mathbf{b}, \hat{\mathbf{t}}^{(\mathbf{n})}\}$ are incrementally applied. The loading magnitude at a loading step or time step n is