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A Moore–Penrose continuation method based on a Schur complement approach for nonlinear finite element bifurcation problems

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ABSTRACT

Continuation methods have proved to be very powerful tools when solving large finite element problems. However, implementation of these methods often require modifications to the standard finite element method. As a finite element code is already very complex, we would like to implement the continuation method as efficiently as possible. In this paper, we present a new implementation technique based on a Schur complement approach for the Moore–Penrose continuation method. This method facilitates the detection of bifurcation points and also enables branch following. Numerical examples will be presented and analyzed using the proposed approach.

1. Introduction

The finite element simulation of very large deformations of hyperelastic materials is still a challenging problem. These problems are generally driven by a loading parameter and it is often observed that for some values of this parameter, the solution varies extremely rapidly due to geometric and/or material non linearities, often leading to the break down of the solution process.

The typical solution strategy is often based on Newton like methods. The loading parameter is set to a given value, the Jacobian matrix stemming from the finite element discretization is constructed, the corresponding linear system is solved to correct the solution and this is repeated until convergence. The loading parameter is then somehow increased ("by hand") and the process is repeated until the total load has been imposed on the structure. One crucial step in terms of computational cost is the solution of the linear systems involving the Jacobian matrix. For moderate size problems, an *LU* decomposition can be used but for very large problems, problem specific preconditioned iterative solvers must be designed and implemented.

In some situations, following the solution branch by increasing heuristically the loading parameter becomes extremely difficult and results in the divergence of the process. This is clearly the case in the neighborhood of limit points or bifurcation points where the Jacobian matrix becomes singular. Numerical continuation methods have proved to be a very powerful tool when dealing with these kinds of problems. They can be roughly divided into two main branches, predictor–corrector methods and piecewise linear methods (see [2]). Both types of methods share many common features and can be numerically implemented in similar ways. However, predictor–corrector methods generally perform best when high accuracy is needed and are thus frequently used in practice. Many different continuation methods exist (see for example [14,11,24,25]), but in this paper, only the Moore–Penrose (also known as Gauss–Newton) continuation method (see [2,13,12]), which is a predictor–corrector method, will be considered.

Nonlinear structural analysis leads invariably to collapse and buckling analysis [7,31]. Buckling is a mathematical instability which is characterized by a sudden failure of the structure when critical loads are reached. The value of these critical loads, which are associated with bifurcation points, are quantities of interests [29,21,30] and correspond to eigenvalues of the system. Detecting such points and following the different solution branches passed these critical loads are thus important and useful to better understand the physical properties of the problem we are solving. The analysis of structural instabilities, which includes the detection of bifurcation points, is generally based on a continuation method (see [11,6,14,18,27,1,22,28]). The implementation of the continuation method presented in this paper will therefore offer an efficient and simpler approach for these analyses.

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In the Moore–Penrose method, the loading parameter becomes an additional unknown of the problem allowing a more precise control of the deformation, increasing its speed whenever possible and slowing it in some critical regions. This is done by modifying the linear system in the Newton method to take care of the additional unknown. This therefore requires a potentially important modification of an existing finite element code. In particular, new iterative solvers must be implemented to solve these increased linear systems.

As many of these problems have thousands or even millions of degrees of freedom, the continuation method should be implemented as efficiently as possible in order to reduce the already high computational cost. In order to achieve this goal, information that has already been calculated for the finite element method should be used whenever possible. This is precisely the main objective of this work. We will present a generalization of the Moore–Penrose continuation method that uses only information already available in a standard finite element code. In particular, all linear systems that have to be solved are based on the classical Jacobian matrix of the problem. Therefore, if an *LU* decomposition of this matrix is available, it can be used directly and if a specific iterative method was used, it can still be used without any modification to follow the solution curve, detect bifurcations and possibly follow various solution branches.

This paper thus presents a new implementation technique for the Moore–Penrose continuation method when applied in a finite element context. This new approach, which takes advantage of information already available, also facilitates the detection of bifurcation points. Section 2 briefly recalls the Moore–Penrose continuation method as well as the classical numerical implementation of this method. Section 3 is devoted to the details of the new implementation technique. Section 4 explains how the approach can be used to easily detect bifurcation points and finally, Section 5 is devoted to the validation of the proposed algorithm. In particular, a study of the classical elastic beam buckling problem will be presented and analyzed.

2. Moore–Penrose continuation method

The finite element discretization of nonlinear elasticity problems leads to nonlinear problems of the form:

$$F(u) = 0$$

where u consists of the degrees of freedom. In general, u is the displacement field, but in the case of mixed formulations, u consists of the degrees of freedom for the displacement and the pressure. In most situations, a loading parameter λ, corresponding to either external forces or prescribed displacements or both, implicitly drives the deformation. For highly nonlinear problems, applying the desired loading will frequently cause a breakdown of the numerical method used to solve this problem. Therefore it is standard practice to gradually increase the value of the parameter until the desired loading, λ_{max}, is attained. Typically, a Newton method is used to solve the nonlinear system. The following steps are therefore repeated until convergence is achieved:

1. Given an initial estimate u^0 and a fixed load λ.
2. Solve the linear system:
   $F'_u(u^k)\,\delta_u^k = F(u^k)$.
3. Update the solution:
   $u^{k+1} = u^k - \delta_u^k$.

where F'_u is the Jacobian matrix of F and δ_u^k is the correction vector. The loading parameter λ is then increased by a certain quantity and the process is repeated until the total load λ_{max} has been imposed. The increment in λ is performed more or less heuristically, depending on the convergence of the Newton method. This is highly inefficient and may result in very small increments or even divergence of the algorithm in the neighborhood of turning points or bifurcation points on the solution curve.

A more efficient approach is to use continuation methods where the loading parameter λ is explicitly introduced in the system of nonlinear equations which is now expressed as:

$$F(u,\lambda) = F(x) = 0 \tag{1}$$

with F a smooth function of $\mathbb{R}^{N+1}$ into $\mathbb{R}^N$. The major difference is that the vector of unknowns, x, now consists of the displacement plus the loading parameter. Starting from a point $x^{(i)} \in \mathbb{R}^{N+1}$ satisfying $F(x^{(i)}) = 0$, and given a vector $v^{(i)}$ tangent to the solution curve at this point, the goal is to follow the curve up to the point where $\lambda = \lambda_{max}$. It is then natural to try to follow the solution curve by first making a prediction step of length h_i in the tangential direction:

$$X^0 = x^{(i)} + h_i v^{(i)} \tag{2}$$

As X^0 is not likely to be a solution of Eq. (1), the Newton method can be used to obtain the next point $x^{(i+1)} \in \mathbb{R}^{N+1}$ on the solution curve. By linearizing Eq. (1) around the prediction point $X^0 = [u^0 \ \lambda^0]^\top$, we can solve:

$$F'_u(X^0)\delta_u + F'_\lambda(X^0)\delta_\lambda = F(X^0)$$

which leads to a rectangular linear system of the form:

$$A(X^0)\delta_x = F(X^0) \tag{3}$$

with $A(X^0) = [F'_u(X^0)\ F'_\lambda(X^0)]$ a rectangular matrix of dimension $n \times (n+1)$ and $\delta_x = [\delta_u \ \delta_\lambda]^\top$ a correction vector of dimension $(n+1) \times 1$.

Assuming that the rows of $A(X^0)$ are linearly independent (i.e. $A(X^0)$ has full rank), which is generally the case since $F'_u(X^0)$ is the Jacobian matrix of the standard finite element method and is therefore invertible, solution of system (3) is given by:

$$\delta_x = A^+(X^0)F(X^0)$$

where A^+ is the Moore–Penrose pseudoinverse of matrix A defined by $A^+ = A^\top(AA^\top)^{-1}$. This therefore leads to the following generalization of the Newton method, which is also called the Moore–Penrose continuation method:

- $X^0 = x^{(i)} + h v^{(i)}$
- For $k = 0, 1, 2, \ldots, k_{max}$
  1. Calculate the Moore–Penrose correction:
     $$\delta_x^k = A^+(X^k)F(X^k) \tag{4}$$
  2. Update the solution vector:
     $X^{k+1} = X^k - \delta_x^k$
  3. If $\|F(X^k)\| \leqslant \varepsilon_F$ and $\|X^{k+1} - X^k\| \leqslant \varepsilon_x$, convergence attained:
     $x^{(i+1)} = X^{k+1}$

  We note that k_{max} represents the maximum number of iterations allowed while ε_F and ε_x are the desired tolerances on F and x respectively.

To obtain the correction δ_x^k in Eq. (4), the Moore–Penrose pseudoinverse A^+ of the matrix $A(X^k) = [F'_u(X^k) \quad F'_\lambda(X^k)]$ is needed. The