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ERROR FREE EVALUATION OF TENSOR FUNCTIONS AND THEIR APPLICATION IN FINITE-STRAIN MODELS

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Many commonly used inelastic material models exhibit highly non-linear behaviour. Solving such problems without appropriate formulation can cause large errors accumulating with each incremental step. One such example is incremental finite strain formulation for multiplicative elastoplasticity which requires the use of time integration, which can accumulate errors if not formulated correctly. One example of inelastic model is Cam-Clay model, which has strain energy expressed with logarithm of deformation tensor and plastic evolution equation with matrix exponential, first derivatives of both functions and only second derivative of matrix logarithm are required. It has been shown that exact integration can be achieved by formulation of evolution equations with tensor functions [1]. Another problem are derivatives of such formulations, which are needed to derive residual and tangent matrices. First derivatives, can in theory, be calculated with finite differences method, but calculating second derivatives is much harder. Library of C subroutines, that return evaluated matrix function and its first and second derivative, which are defined with machine precision on their definition area, can be prepared in advance, thus they can be considered as elementary functions. Consequently the formulation of complex non-linear problems using matrix functions can be be greatly simplified and its results up to machine precision accurate.

The calculation of a general matrix function of general $n \times n$ matrix is not a simple task. Moler [2] has shown several possibilities of calculating of matrix exponential. There is no general method which is completely satisfactory, additionally in computational mechanics, derivatives of matrix functions must be known, to derive residual and tangent matrix. Most commonly the matrix functions are calculated using its spectral decomposition or its series expansion [1]. Spectral decomposition presents another problem of determining eigenvalues of a matrix, because they exhibit ill-conditioning in vicinity of multiple equal eigenvalues. Since our interests lies with application in solid mechanics, we can limit ourselves to matrices of dimension 3×3. In this case closed form eigenvalues can be formulated analyticity with trigonometric functions.

In this work, we will derive matrix functions by differentiating a scalar generating function of the eigenvalues of the matrix as shown in [3]. The presented approach will be applied to various matrix functions, specifically on matrix exponential, logarithm, square, power and power series. Development of the closed form representations of mentioned matrix functions and their first and second derivative will be shown for 3×3 matrix where eigenvalues can be analytically defined. When eigenvalues are exactly equal it is relatively easy to derive closed form representation, but when they are nearly equal, ill-conditioning requires complex asymptotic expansion of generating function. Closed form representations of matrix functions and its first and second derivatives were derived using AceGen code generation system [4]. C library of subroutines mentioned closed form matrix functions along with their first and second derivative has been created and is available for use in general finite element environment.

Accuracy of derived closed-form matrix functions will be compared with its series expansion in the vicinity of multiple eigenvalues. Errors are in range of machine precision for all matrix functions and their first derivatives, while errors of the second derivatives are in the range of 10^{-10}. Efficiency of derived closed-form representations will be shown on an example of Ogden material and modified Cam-Clay soil model. Strain energy of the first can be expressed with matrix power sum while strain energy of the second is expressed with matrix logarithm and the plastic evolution equation with matrix exponential. Presented closed form representations of matrix function enables accurate, stable and numerically effective calculation of finite strain material models. Described procedure can be generalized to any matrix function.

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