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

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Abstract. In our work a formulation that leads to accurate and efficient solution of inelastic material models that exhibit highly non-linear behaviour will be presented. Solving such problems without appropriate formulation can cause large errors accumulating with each incremental step. It has been shown that accumulative time integration of evolution equations can be achieved by formulation of discritized equations with tensor functions. Additionally in computational mechanics, derivatives of matrix functions must be known, to derive residual and tangent matrix. We will present method to compute numerically efficient closed-form representation of matrix functions for 3×3 matrices with real eigenvalues and its first and second derivative. Matrix functions will be obtained by differentiating an appropriate scalar generating function using automatic differentiation procedure. Accuracy of derived closed-form matrix functions will be compared with its series expansion in the vicinity of multiple eigenvalues where functions are severely ill conditioned. Errors of derived closed-form matrix functions and their first derivatives are in range of machine precision, while errors of the second derivatives are in the range of 10^{-10}. Efficiency of derived closed-form representations will be shown on a numerical example of Ogden material model. Ogden model will be compared with elements which contain appropriate strain energy of Neo-Hooke and Mooney-Rivlin material models. An example of modified Cam-Clay soil model will also be shown. 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.

1 INTRODUCTION

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. It has been shown that exact integration can be achieved by formulation of evolution equations with tensor functions [1, 2]. Additionally in computational mechanics, derivatives of matrix functions must be known, to derive residual and tangent matrix. First derivatives, can in theory, be calculated with finite differences method, but calculating second derivatives is much harder. Strain energy function for most finite strain elements is sometimes expressed with matrix functions. One example of inelastic material is Ogden material which is usually expressed as sum of powers of stretches which requires spectral decomposition of deformation tensors. Model can be alternatively expressed with a finite series of matrix power sums. Solution procedure requires also first and second derivatives of matrix power. Another 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. Procedure requires first and second derivatives of matrix logarithm and only first derivative of matrix exponential.

If 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, matrix functions could be considered as elementary functions. Consequently the formulation of complex non-linear problems using matrix functions can 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 [3] has shown several possibilities of calculating of matrix exponential. There is no general method which is completely satisfactory that would meet all demands. Most commonly the matrix functions are calculated using its spectral decomposition or its series expansion [1]. Spectral decomposition introduces additional another problem of accurately determining eigenvalues of a matrix, because they exhibit ill-conditioning in vicinity of multiple equal eigenvalues. This areas require special treatment. Among other possibilities shown by Moler, matrix function can be obtained by differentiating a scalar generating function of the eigenvalues of the matrix [4]. 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. 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.

2 COMPUTATION OF CLOSED FORM MATRIX FUNCTIONS AND ITS DERIVATIVES

Development of the closed form representations of matrix functions and their first and second derivative will be shown for 3×3 matrix where eigenvalues can be analytically defined. Closed form representations of mentioned matrix functions and its first and second derivatives will be derived using *AceGen* code generation system [5] and *Mathematica*.

2.1 Deriving generating functions

Previously outlined method can be applied to arbitrary matrix function $\mathcal{F}(\mathbf{A})$. Matrix function can be formulated as derivative of appropriate generating function $G(\mathbf{A})$ with respect to transposed matrix $F(\mathbf{A}) = \frac{\partial G(\mathbf{A})}{\partial \mathbf{A}^T}$, therefore first task is to determine generating function. By Lu [4], generating function $G(\mathbf{A}) = \sum_i g(\lambda_i)$ is defined as sum of auxiliary functions $g(\lambda_i) = \int f(\lambda_i) d\lambda_i$, which are integrals of equivalent scalar function $f(\lambda_i)$ applied on eigenvalues of matrix $\mathbf{A}$. Applying this on matrix power ($G_{\mathcal{P}}$), power sum ($G_{\mathcal{S}}$) and logarithm ($G_{\mathcal{L}}$), their generating functions can easily be obtained as functions of eigenvalues:

$$G_{\mathcal{P}} = \sum_{i=1}^{3} \frac{\lambda_i^{\eta+1}}{\eta+1}, \quad G_{\mathcal{L}} = \sum_{i=1}^{3} (-\lambda_i + \lambda_i \log(\lambda_i)), \quad G_{\mathcal{S}} = \sum_{k=1}^{n} \xi_k G_{\mathcal{P}}(\mathbf{A}, \eta_k), \tag{1}$$

To evaluate the generating functions, eigenvalues λ_i of matrix $\mathbf{A}$ must first be determined. The procedure to determine eigenvalues for 3×3 matrix is given by [2]. First matrix $\mathbf{A}$ is split into volumetric $\mathbf{A}'' = a\mathbf{I}$ and deviatoric $\mathbf{A}' = \mathbf{A} - \mathbf{A}''$ parts. Where $a = \frac{1}{3} tr(\mathbf{A})$ represents the eigenvalues of volumetric part. The characteristic polynomial of matrix $\mathbf{A}'$ is written in the following form

$$(\lambda')^3 - \frac{1}{2} p\lambda' - q = 0, \qquad p = tr(\mathbf{A}'\mathbf{A}'), \qquad q = \det \mathbf{A}'. \tag{2}$$

The eigenvalues λ_i' of $\mathbf{A}'$ can be written analytical using trigonometric functions as:

$$\lambda_1' = t\cos\phi, \quad \lambda_2' = t\cos\left(\phi - \frac{2\pi}{3}\right), \quad \lambda_3' = t\cos\left(\phi + \frac{2\pi}{3}\right), \tag{3}$$

where $t = \sqrt{\frac{2}{3}}\sqrt{p}$, $r = 3\sqrt{6}\,\frac{q}{p^{3/2}}$ and $\phi = \frac{1}{3}\arccos(r)$. The eigenvalues of matrix $\mathbf{A}$ can then be defined as $\lambda_i = a + \lambda_i'$. The generating function $G_{\square}$ can now be expressed in terms of the eigenvalues of $\mathbf{A}'$ and with trace of $\mathbf{A}$. Given equations are analytical, however in the vicinity of multiple equal eigenvalues, the equations become singular. The nature of eigenvalues can be determined from equation $\Delta = \frac{1}{2}p^3 - 27q^2$. The sign of Δ determines the nature of eigenvalues. Since application in solid mechanics is considered, $\Delta > 0$ must hold to ensure $\mathbf{A}$ has three distinct real eigenvalues. This condition is equivalent to condition $-1 \geq r \leq 1$ and also implies condition $p \geq 0$. When p and r are approaching

boundary values, the equations become singular. As seen in Figure 1 small perturbation over ± 1 causes eigenvalues to become complex. These two critical cases require special treatment, which is presented below.

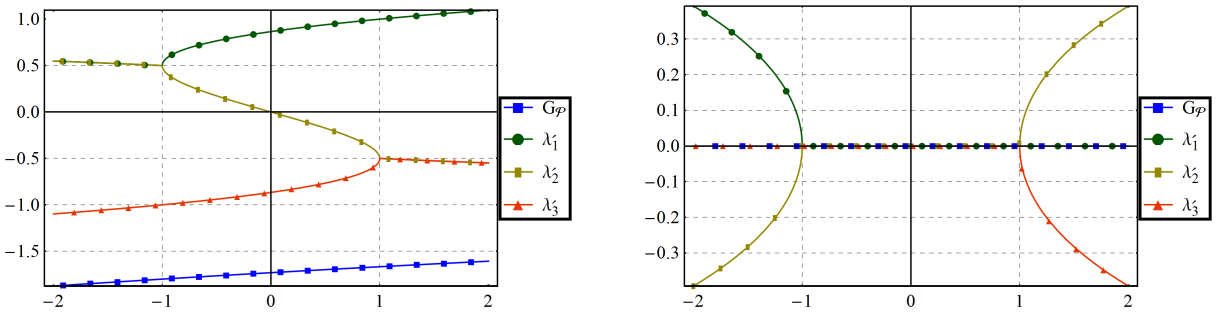


Figure 1: Real and imaginary parts of eigenvalues λ_i and genertating function $G_{\mathcal{P}}$

For the first special case, where the parameter p reaches 0, the generating function must be expanded around $p = 0$. It can be easily shown that q also approaches zero, therefore a multivariate asymptotic expansion of G around $p = 0$ and $q = 0$ is considered. The expansion when $p < \varepsilon_p$ follows as:

$$G_p = \sum_{n_p=0}^{\infty} \sum_{n_q=0}^{\infty} \frac{\partial^{n_p+n_q} G}{\partial p^{n_p} \partial q^{n_q}}\bigg|_{\substack{p\to 0 \\ q\to 0}} \frac{p^{n_p} q^{n_q}}{n_p! n_q!} \tag{4}$$

It turns out that choosing maximum fifth order derivative of G, this means $(n_p + n_q)_{max} = 5$, the results are satisfactory for sufficiently small ε_p. If we apply (4) on $G_{\mathcal{P}}$ we get series expansion for matrix power generating function for the case when $p \to 0$:

$$\begin{aligned} G_{\mathcal{P},\mathrm{p}} = a^\eta \Bigg(& \frac{3a}{\eta+1} + \frac{\eta}{2a} \Bigg(p + \frac{\eta-1}{a} \Bigg(q + \frac{\eta-2}{24a} \Bigg(p^2 + \frac{\eta-3}{a} \cdot \\ & \cdot \Bigg(pq + \frac{\eta-4}{5a} \Bigg(\frac{p^3}{12} + q^2 + \frac{\eta-5}{6a} \Bigg(\frac{p^2 q}{2} + \frac{\eta-6}{7a} \Bigg(\frac{p^4}{32} + pq^2 + q\frac{\eta-7}{4a} \cdot \\ & \cdot \Bigg(\frac{p^3}{8} + \frac{q^2}{3} + q\frac{\eta-8}{12a} \Bigg(\frac{p^2}{2} + q\frac{\eta-9}{15a} \Bigg(p + q\frac{\eta-10}{22a} \Bigg) \Bigg) \Bigg) \Bigg) \Bigg) \Bigg) \Bigg) \Bigg) \Bigg) \Bigg) \Bigg) \end{aligned} \tag{5}$$

For the second special case, where the parameter r reaches ± 1, the generating function is expanded around $r = \pm 1$. The expansion follows as:

$$G_r = \sum_{n_r=0}^{\infty} \frac{\partial^{n_r} G}{\partial r^{n_r}}\bigg|_{r\to\pm 1} \frac{(r+s_r)^{n_r}}{n_r!}, \quad \text{where} \quad s_r = \begin{cases} 1 & \text{if } r < -1 + \varepsilon_r, \\ -1 & \text{if } r > 1 - \varepsilon_r, \end{cases} \tag{6}$$

If we apply (6) on $G_{\mathcal{P}}$ we get series expansion for matrix power generating function for the second special case when $r \to \pm 1$. :

$$\begin{aligned}
G_{\mathcal{P}}|_{r=\pm 1} &= (s_r t(p_2 - p_1) + a(p_1 + 2p_2))(\eta + 1), \\
\left.\frac{\partial G_{\mathcal{P}}}{\partial r}\right|_{r=\pm 1} &= t(2s_r a(p_1 - p_2) + t((3\eta - 1)p_2 + p_1))(18 p_2^{-\eta} s_r), \\
\left.\frac{\partial^2 G_{\mathcal{P}}}{\partial r^2}\right|_{r=\pm 1} &= t(t(t(t(s_r t((3\eta - 8)p_1 + (8 - 9(\eta - 3)(\eta - 2)\eta)p_2) \\
&\quad + 2(9\eta - 20)p_1 a + (9(\eta - 3)\eta(\eta + 2) + 40)p_2 a) \\
&\quad + 12 s_r a^2 (3\eta(-\eta p_2 + p_1 + p_2) + 4(p_2 - p_1))) \\
&\quad + 8a^3((3\eta + 4)p_1 + (9\eta - 4)p_2)) + 64 s_r a^4 (p_1 - p_2)) \\
&\quad /(1944 p_1^{-\eta} p_2^{-\eta+3}),
\end{aligned} \tag{7}$$

where $p_1 = (-s_r t + a)$ and $p_2 = (s_r t/2 + a)$. The generating function can then be written for all special regions for all matrix functions as:

$$\mathcal{G} = \begin{cases} G & p \geq \varepsilon_p \ \wedge \ r \geq -1 + \varepsilon_r \ \wedge \ r \leq 1 - \varepsilon_r, \\ G_p & p < \varepsilon_p, \\ G_r & r < -1 + \varepsilon_r \ \wedge \ r > 1 - \varepsilon_r, \end{cases} \tag{8}$$

The matrix function and its derivatives with respect to matrix $\mathbf{A}$ can be formulated with automatic differentiation based formulation with the help of software tool *AceGen*.

$$\mathcal{F}(\mathbf{A}) = \frac{\hat{\delta}\mathcal{G}(\mathbf{A})}{\hat{\delta}\mathbf{A}^T}, \ \delta\mathcal{F}(\mathbf{A}) = \frac{\partial \mathcal{F}(\mathbf{A})}{\partial \mathbf{A}} = \frac{\hat{\delta}\mathcal{F}(\mathbf{A})}{\hat{\delta}\mathbf{A}} \text{ and } \frac{\partial^2 \mathcal{F}(\mathbf{A})}{\partial \mathbf{A}^2} = \frac{\hat{\delta}(\delta\mathcal{F}(\mathbf{A}))}{\hat{\delta}\mathbf{A}}, \tag{9}$$

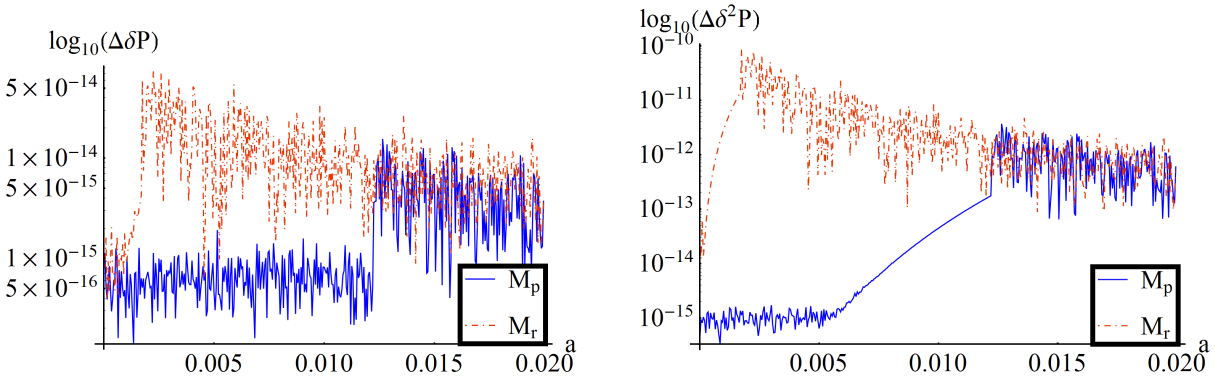
following notation of [6], the $\frac{\hat{\delta}\square}{\hat{\delta}\square}$ is automatic differentiation operator. With this procedure arbitrary matrix functions can be written, such as matrix exponential, logarithm, power, square root and others. Matrix functions are through article labelled as: Matrix power $\mathcal{P}(\mathbf{M}, \eta)$, finite matrix power sum $\mathcal{P}_{\mathrm{s}}(\mathbf{M}, \boldsymbol{\xi}, \boldsymbol{\eta})$, matrix logarithm $Log(\mathbf{M})$, matrix exponential $Exp(\mathbf{M})$, where η is an arbitrary exponent, $\boldsymbol{\eta}$ is a vector of arbitrary exponents and $\boldsymbol{\xi}$ is a vector of arbitrary factors.

3 TEST OF ACCURACY OF CLOSED FORM MATRIX IMPLEMENTATION OF MATRIX POWER

Closed form matrix power or $\mathcal{P}(\mathbf{M}, \frac{1}{2})$ will be compared with truncated series approximation of matrix power labelled as $\bar{\mathcal{P}}(\mathbf{M}, \frac{1}{2})$. The chosen tolerances for regions $|r| > 1 - \varepsilon_r$ and $p < \varepsilon_p$, where the series expansion is required are $\varepsilon_r = 10^{-3}$ and $\varepsilon_p = 10^{-4}$. The numerical accuracy of closed form solution will be tested on matrices $\mathbf{M}_p$ and $\mathbf{M}_r$, which characteristic polynomial is located on boundary regions.

$$\mathbf{M}_p = \frac{1}{8}\begin{bmatrix} 3a+4 & 3a & \sqrt{6}a \\ 3a & 3a+4 & \sqrt{6}a \\ \sqrt{6}a & \sqrt{6}a & 2(a+2) \end{bmatrix} \quad \mathbf{M}_r = \frac{1}{8}\begin{bmatrix} 3a+\frac{22}{5} & 3a-\frac{2}{5} & \sqrt{6}a \\ 3a-\frac{2}{5} & 3a+\frac{22}{5} & \sqrt{6}a \\ \sqrt{6}a & \sqrt{6}a & 2(a+2) \end{bmatrix}$$

Values a are increased from 0 to 0.02 in 400 steps. The difference between closed form and truncated series implementation ($\Delta\mathcal{P} = ||\mathcal{P} - \bar{\mathcal{P}}||$) and their derivatives is monitored.



(a) Error of first derivative

(b) Error of second derivative

Figure 2: Accuracy of first and second derivatives of matrix power

On Figure 2 the accuracy of derivatives of matrix function $\mathcal{P}$ can be observed. The results show that the error $\Delta\mathcal{P}$ is in all cases in range 10^{-15}. With higher derivatives, the error increases. For $\mathbf{M}_p$ the largest error of first derivative is in range of 10^{-14}, and of the second 10^{-12}. For $\mathbf{M}_r$ the largest error of first derivative is in range of 5×10^{-14}, and of the second 10^{-10}. The jumps between different regions of functions G_p and G_r with $a = 0.0122$ for $\mathbf{M}_p$ and between G_r and G with $a = 0.00175$ for $\mathbf{M}_r$ can be observed from figure 2. Similar observations can be made for matrix logarithm.

4 APLICATION OF FINITE MATRIX POWER SUM ON OGDEN MATERIAL MODEL

Ogden material model is on of the most general hyperelastic models. With appropriate choice of material parameters it can describe models such as Neo-Hooke, Mooney-Rivlin, Ogden and Ogden-Stoaker materials for rubber and foams among others. The general form of the Ogden material strain potential is

$$W = \sum_{k=1}^{n} \frac{\mu_k}{\alpha_k}(\lambda_1^{\alpha_k} + \lambda_2^{\alpha_k} + \lambda_3^{\alpha_k} - 3) + g(J), \tag{10}$$

where $g(J)$ is appropriate volumetric part of potential, different possibilities for $g(J)$ are given in [7]. μ_k are partial shear moduli and α_k are powers of main stretches λ_i. Total

shear modulus can be calculated from equation $\sum_{k=1}^{n} \frac{1}{2}\mu_k\alpha_k = \mu$. Formulation expressed with eigenvalues is unfavourable, so we want to write the corresponding matrix function whose generating function will be the potential (10) itself. Such function is a finite matrix power sum derived in previous section.

4.1 Implementation of Ogden material model

With the choice of factors $\boldsymbol{\xi} = \boldsymbol{\mu}/2$ and powers $\boldsymbol{\eta} = \boldsymbol{\alpha}/2 - 1$, the Ogden potential (10) can be expressed with the generating function of matrix power sum as

$$W = \sum_{k=1}^{n} \frac{\mu_k}{\alpha_k} \left(\sum_{i=1}^{3} \lambda_i^{\alpha_k} - 3 \right) + g(J) = \mathcal{G}_{\mathcal{PS}} \left(\bar{\boldsymbol{C}}, \frac{\boldsymbol{\alpha}}{2} - 1, \frac{\boldsymbol{\mu}}{2} \right) - \sum_{k=1}^{n} \frac{3\mu_k}{\alpha_k} + g(J) = \bar{W} + g, \tag{11}$$

where $\bar{\boldsymbol{C}} = J^{-\frac{2}{3}}\boldsymbol{C}$ is a deviatoric part of right Cauchy-Green deformation tensor $\boldsymbol{C} = \boldsymbol{F}^T.\boldsymbol{F}$. From this expression the residual of an arbitrary finite element with Ogden model can be expressed using matrix function $\mathcal{P}_\mathrm{s}$:

$$\begin{aligned} \mathbf{R}_e(\mathbf{p}_e) = \frac{\partial W}{\partial \mathbf{p}_e} = \frac{\partial \bar{W}}{\partial \mathbf{p}_e} + \frac{\partial g}{\partial \mathbf{p}_e} = \frac{\partial \bar{W}}{\partial \bar{\boldsymbol{C}}} \frac{\partial \bar{\boldsymbol{C}}}{\partial \mathbf{p}_e} + \frac{\partial g}{\partial \mathbf{p}_e} = \\ = \mathcal{P}_\mathrm{s} \left(\bar{\boldsymbol{C}}, \frac{\boldsymbol{\alpha}}{2} - 1, \frac{\boldsymbol{\mu}}{2} \right) \cdot \frac{\partial \bar{\boldsymbol{C}}}{\partial \mathbf{p}_e} + \frac{\partial g}{\partial \mathbf{p}_e} = \left. \frac{\hat{\delta} W}{\hat{\delta} \mathbf{p}_e} \right|_{\frac{D\bar{W}}{D\mathbf{p}_e} = \mathcal{P}_\mathrm{s}\left(\bar{\boldsymbol{C}}, \frac{\boldsymbol{\alpha}}{2} - 1, \frac{\boldsymbol{\mu}}{2} \right)} \end{aligned} \tag{12}$$

where $\mathbf{p}_e$ is the vector of degrees of freedom of finite element. Tangent matrix of finite element can be written as $\mathbf{K}_e(\mathbf{p}_e) = \frac{\hat{\delta}\mathbf{R}_e}{\hat{\delta}\mathbf{p}_e}$.

4.2 The efficiency of element with Ogden potential

The efficiency of derived matrix power sum will be compared with finite elements for Neo-Hooke and Mooney-Rivlin models formulated with their own potential in a classical way. Neo-Hooke potential model is written as:

$$W_{\mathrm{NH}} = \frac{\mu}{2}(\mathrm{tr}(\bar{\boldsymbol{C}}) - 3) + \frac{\kappa}{4} \left(J^{-2} - 2\log(J) - 1 \right) \tag{13}$$

and Mooney-Rivlin potential as:

$$W_{\mathrm{MR}} = \frac{\mu_1}{2}(\mathrm{tr}(\bar{\boldsymbol{C}}) - 3) + \frac{\mu_2}{2} \left(\frac{1}{2} \left((\mathrm{tr}(\bar{\boldsymbol{C}}))^2 - \mathrm{tr}(\bar{\boldsymbol{C}}.\bar{\boldsymbol{C}}) \right) - 3 \right) + \frac{\kappa}{4} \left(J^{-2} - 2\log(J) - 1 \right) \tag{14}$$

where J is Jacobian of deformation gradient $\boldsymbol{F}$, μ and κ shear and stiffness moduli. This models are reduction of Ogden material model when $\boldsymbol{\alpha} = \{2\}$ and $\boldsymbol{\mu} = \{\mu\}$, $\boldsymbol{\alpha} = \{2, -2\}$ and $\boldsymbol{\mu} = \{\mu_1, \mu_2\}$. For $g(J)$ the chosen function is $g(J) = \frac{\kappa}{4} \left(J^{-2} - 2\log(J) - 1 \right)$ from [7].

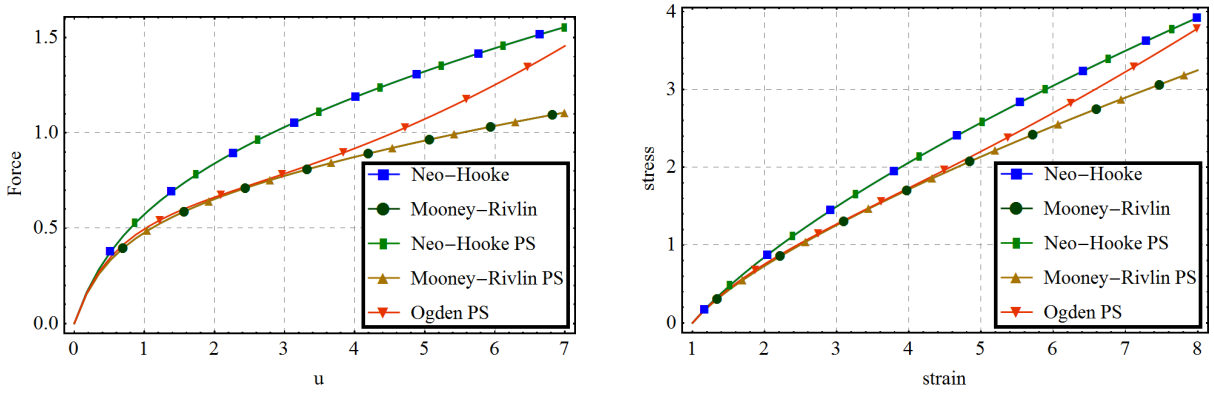
Table 1: material characteristic of considered materials

Material	$\boldsymbol{\alpha}$	$\boldsymbol{\mu}$
Neo-Hooke	$\{2\}$	$\{0.4225\}$
Mooney-Rivlin	$\{2, -2\}$	$\{0.24, -0.1825\}$
Ogden's material	$\{1.3, 5, -2\}$	$\{0.63, 0.0012, -0.01\}$

With Ogden model with choice of parameters $\boldsymbol{\alpha}$ and $\boldsymbol{\mu}$ three materials will be described as shown in Table 1. The shear moduli are chosen in a way that for all models results in equal total shear modulus $\mu = \sum_{k=1}^{n} \frac{\mu_k \alpha_k}{2} = 0.4225$. The compression modulus is $\kappa = 0.915417$ ($\nu = 0.3$) for all examples. For each considered material the cube of dimension $1 \times 1 \times 1$, discretized with $24 \times 24 \times 24$ elements. In x direction the displacement $u_x = 7$ units is applied, in directions y and z the displacement is unconstrained.

Table 2: The comparison of numerical efficiency of elements

Example	N-H	M-R	N-H -PS	M-R -PS	Ogd -PS
Total simulation time (s)	542.4	521.9	610.8	628.3	741.4
Normed single iteration time	1	1.02	1.13	1.19	1.28
Normed linear solver time	1	0.95	1.	0.97	1.07
Normed **K** and **R** assembly time	1	1.17	2.58	3.43	4.51
Code size (KB)	26881	28808	33917	33917	33917
Number of equations	500	544	654	654	654



(a) displacement - force

(b) stretch- stress

Figure 3: The comparrisson of different models. First and second are classical potentials (13,14), last three are expressed with matrix power sum (12).

The growth of the assembly time of tangent matrix $\mathbf{K}$ and the residual $\mathbf{R}$ is monitored with each added term in power sum. In Table 2, the effectiveness of the constructed finite element model with Ogden model and Neo-Hooke and Mooney-Rivlin materials are compared. As expected, the latter are faster and smaller. Assembly time of $\mathbf{K}$ and $\mathbf{R}$ for Ogden model with one term of matrix power is for factor 2.6 longer. It represents around 15 % of the time needed for one iteration therefore the average time needed for one iteration is longer by only 13 %. By adding terms the time required for one iteration increases by 7 to 9 % for each added term. Ogden model with one power sum returns an identical results to the Neo-Hooke's. The difference of their $\mathbf{K}$ and $\mathbf{R}$ matrices is of the order of 10^{-15}. Ogden model with two terms yields identical results as Mooney-Rivlin model. In Figure 3 the stresses and forces can be seen with respect to stretches and displacements. The curves are in good agreement up to stretch 1.5, then the curve of other models begin to move away from the Neo-Hooke material.

5 APPLICATION ON MODIFIED CAM-CLAY MODEL

Modified Cam-Clay model is basic model for soil, whose volumetric strain energy is expressed with logarithm of stretches and its plastic yield surface is ellipsoid. The model will be formulated according to Ortiz [8]. Strain energy of Cam-Clay model can be written as:

$$W = W^{e,vol} + W^{e,dev} = \frac{\kappa}{2}(\theta_{\mathrm{e}})^2 + \mu\|\bar{\boldsymbol{e}}_{\mathrm{e}}\|^2 \tag{15}$$

where κ in μ are compression and shear modulus. $\theta_{\mathrm{e}} = log(J_{\mathrm{e}})$ is logarithm of Jacobian of elastic deformation gradient $\boldsymbol{F}_{\mathrm{e}}$. J_{e} is $det(\boldsymbol{b}_{\mathrm{e}})^{\frac{1}{2}}$ where b_{e} is Left Cauchy-Green deformation tensor. The $\bar{\boldsymbol{e}}_{\mathrm{e}}$ is deviatoric part of elastic Eulerian logarithmic deformation tensor $\boldsymbol{e}_{\mathrm{e}}$ an can be calculated directly from $\boldsymbol{b}_{\mathrm{e}}$ as $\bar{\boldsymbol{e}}_{\mathrm{e}} = \frac{1}{2}Log(J_{\mathrm{e}}^{-\frac{2}{3}}\boldsymbol{b}_{\mathrm{e}})$. The yield surface is given as

$$\mathcal{F} = q^2 + \alpha^2 p(p - p_c) \tag{16}$$

where p_c is consolidation pressure, $p = \frac{1}{3}tr(\boldsymbol{\sigma})$ are Cauchy hydrostatic pressures and $q = \sqrt{\frac{2}{3}}\|\boldsymbol{\sigma'}\|$, $\boldsymbol{\sigma'} = \boldsymbol{\sigma} - p\mathbf{I}$ are the deviatoric stresses and α defines the slope of critical state line. Cauchy stress $\boldsymbol{\sigma} = \boldsymbol{\tau}/J$ can be derived from Kirchoff stress $\boldsymbol{\tau} = 2\boldsymbol{b}_{\mathrm{e}}\frac{\partial W}{\partial \boldsymbol{b}_{\mathrm{e}}} + Jp_0$, which can be derived with differentiation of potential with respect to $\boldsymbol{b}_{\mathrm{e}}$. p_0 is initial pressure in soil.

5.1 Evolution equation, flow rule and hardening

Evolution equation for Cam Clay is given by Callari [9] as: $-\frac{1}{2}\mathcal{L}_v\boldsymbol{b}_{\mathrm{e}} = \Delta\dot{\gamma}\mathbf{n}\boldsymbol{b}_{\mathrm{e}}$, where $\mathcal{L}_v\boldsymbol{b}_{\mathrm{e}}$ is Oldroyd derivative of $\boldsymbol{b}_{\mathrm{e}}$ and $\mathbf{n} = \frac{\partial \mathcal{F}}{\partial \boldsymbol{\tau}}$ is direction of flow. Evolution law can then

be written in discritized form as:

$$\boldsymbol{b}_{\mathrm{e}} = \exp(-2(\gamma - \gamma_n)\mathbf{n}/n_f)\mathbf{F}\,\boldsymbol{C}_{\mathrm{p},n}^{-1}\boldsymbol{F}^{\mathrm{T}}, \tag{17}$$

where the only difference from classical isotropical plasticity is norm n_f. Ortiz states, that $\mathbf{n}$ must satisfy $\frac{1}{\alpha^2}tr(\mathbf{n})^2 + \frac{2}{3}\|\mathbf{n}'\| = 1$ and because of this demand the factor $n_f = \sqrt{\frac{1}{\alpha^2}tr(\mathbf{n})^2 + \frac{2}{3}\|\mathbf{n}'\|}$ is introduced. Hardening law is given as $p_{\mathrm{c}} = p_{\mathrm{ref}}\exp(\frac{\theta^{\mathrm{p}}}{\theta^{\mathrm{p}}_{\mathrm{ref}}})$. p_{ref} is reference consolidation pressure and $\theta^{\mathrm{p}}_{\mathrm{ref}}$ reference logarithmic volumetric strain, which can also be estimated as $\theta^{\mathrm{p}}_{\mathrm{ref}} = -\frac{\lambda}{v_{\mathrm{ref}}}$, where λ is virgin compression modulus of soil and v_{ref} reference specific volume. Indices $\square_n$ apply on the quantity from previous step. It is beneficiary for internal variables to be expressed with $\boldsymbol{C}_{\mathrm{p}}^{-1}$, because $\boldsymbol{b}_{\mathrm{e}} = \boldsymbol{F}\boldsymbol{C}_{\mathrm{p}}^{-1}\boldsymbol{F}^{\mathrm{T}}$ is its *"push-forward"*.

5.2 Implementation of Cam-Clay material model

The implementation of Cam-Clay model in finite element environment is straight forward when automatic coding an analytical differentiation based formulation is used. Reader is referred to [2], where application of matrix exponential in isotropic plastic models is discussed.

5.3 APPLICATION ON MODIFIED CAM-CLAY MODEL ON EXAMPLE

Soil will be modelled for two different type of soils, one with normally consolidated and one with over consolidated properties. Axisymmetric Cam-Clay quadrilateral element formulated with matrix logarithm and plastic flow with matrix exponential will be compared with results of small strain explicit model by Potts [10] on one element of dimension 1×1. The displacement on top surface is prescribed and displacement on vertical side is movement is free.

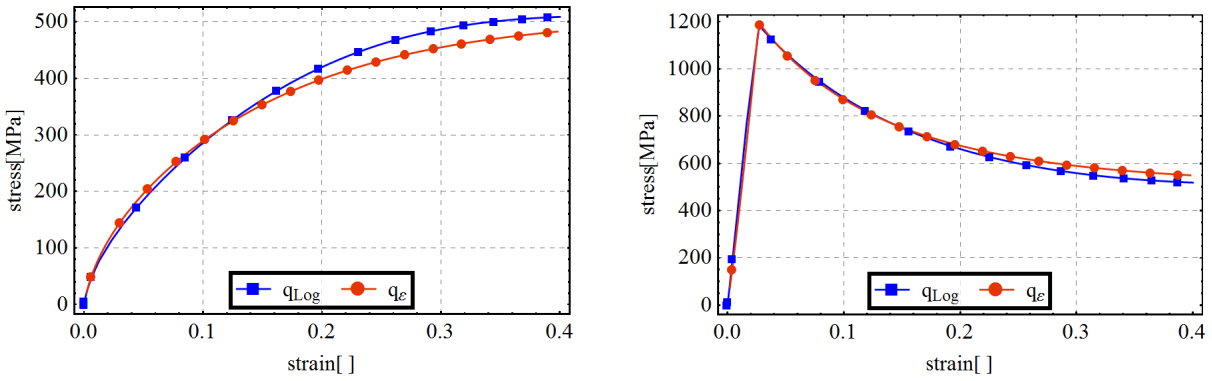
Table 3: Material parameters for soil models

Parameter	κ(MPa)	μ(MPa)	p_{ref}(MPa)	$\theta^{\mathrm{p}}_{\mathrm{ref}}$	p_{c0} (MPa)	$\phi(^\circ)$
Value NC	21360	20000	-200	-0.106	-200	30
Value OC	21360	20000	-1851	-0.132	-200	30

Results are in good agreement for small strains, then they start to diverge around strain 0.15 as seen in figure 4.

6 CONCLUSIONS

In this work, we have demonstrated a method for deriving an arbitrary closed form matrix function and its first and second derivatives of matrix of order 3×3 with real eigenvalues. They can be derived using automatic differentiation of generating functions. It turns out that the approximation of derived matrix functions is very accurate also in



(a) normally consolidated (b) over consolidated

Figure 4: Normaly consolidated and overconsolidated soil (E_{xx} - q)

the vicinity of multiple equal eigenvalues. Error of matrix function is of the order of 10^{-15}. Error of its first derivative is maximum 5×10^{-14} and error of the second derivative is maximum 10^{-10}. Library of C subroutines, that returns evaluated matrix functions (at the time they are called) and their first and second derivatives, which are defined with machine precision on their definition area, have been prepared in advance using *AceGen* code generation system. Thus they can be considered as elementary functions. Consequently the formulation of complex non-linear problems using matrix functions is greatly simplified and its results up to machine precision accurate.

Using a matrix power sum the hyper hyper-elastic Ogden type material model was derived. By choosing the appropriate material parameters it can be used to calculate the Neo-Hooke (one article), Mooney-Rivlin (two articles), Ogden material (three articles). For comparison, we have taken the Neo-Hooke and Mooney-Rivlin material models derived classically and the difference in efficiency between them is minimal. The results of direct implementation and implementation with matrix function are identical, the **K** and **R** assembly time, was longer for factor 2.6 For each added term in Ogden material model definition, this factor is increased by about 1 The size of the source code of the element is larger than the direct implementation for 26%. From the obtained results it can be concluded that the derived closed form matrix function is efficient and accurate.

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