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The Development of Unique Orthogonal Rotation Tensor Algorithm in the LLNL-DYNA3D for Orthotropic Materials Constitutive Model

M.K. Mohd Nor

Faculty of Mechanical Engineering and Manufacturing, Tun Hussein Onn University, Beg Berkunci 101 Parit Raja, Batu Pahat, 86400, Johor, Malaysia

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ABSTRACT

A unique orthogonal rotation tensor was defined and implemented into the Lawrence Livermore National Laboratory-DYNA3D code in this paper. This tensor is vital for the implementation work of a newly formulated constitutive model proposed by M. K. Mohd Nor, to ensure the analysis was precisely integrated in the isoclinic configuration. The implementation of this unique orthogonal rotation tensor into the LLNL-DYNA3D was performed by referring to three theorems; the deformation gradient **F**is invertible, the plastic stretch **U**is symmetric and positive definite and finally the rotation tensor$\widehat{\mathbf{R}}$is assumed orthogonal hence$\widehat{\mathbf{R}}^{-1} = \widehat{\mathbf{R}}^{T}$. The subroutine chkrot93 was adopted to check the accuracy of the proposed algorithm to calculate a proper rotation tensor $\widehat{\mathbf{R}}$. This subroutine requires only the candidate rotation tensor $\widehat{\mathbf{R}}$ in a matrix form as an input, and one value of output named IERR is generated. The accuracy of the proposed algorithm to define a unique orthogonal rotation tensor was tested and validated with the uniaxial tensile test of reversed loading and Plate Impact test of orthotropic materials that have so much application in real world practices. The results obtained in each material direction proved the accuracy of the rotation tensor algorithm to calculate a proper rotation tensor and provide a good agreement for orthotropic materials throughout the analysis.

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INTRODUCTION

The development of a unique orthogonal rotation tensor in the LLNL-DYNA3D is required to support the integration of a newly constitutive model proposed by M. K. Mohd Nor (2013). The formulation that was proposed to modelshockwave propagation in orthotropic materials was developed in the isoclinic configuration$\overline{\mathbf{\Omega}}_i$and provides a unique treatment for elastic and plastic anisotropy. The important features of this constitutive model are the multiplicative decomposition of the deformation gradient **F**and a Mandel stress tensor combined with the new stress tensor decomposition generalized for orthotropic materials (2013). The formulation of new Mandel stress tensor $\widehat{\mathbf{\Sigma}}$defined in the isoclinic configuration wasgivenby:

$$\widehat{\mathbf{\Sigma}} = \det(\mathbf{F}) \cdot \widehat{\mathbf{R}}^{T} \cdot \left(\mathbf{S} + \frac{\sigma\psi}{\psi\psi} \cdot \boldsymbol{\psi}\right) \cdot \widehat{\mathbf{R}}^{-T}. \qquad (1)$$

where $\boldsymbol{\psi}$, $\widehat{\mathbf{R}}$,$\boldsymbol{\sigma}$and**S** define the direction of the new volumetric axis in stress space, the orthogonal rotation tensor, the Cauchy stress and the deviatoric stress tensor respectively. In the LLNL-DYNA3D code, all material models are given with the Cauchy stress $\boldsymbol{\sigma}$ and the rate of deformation **D** tensors at current configuration $\mathbf{\Omega}_t$. Therefore, according to the proposed formulation, these tensors must be pulled back to the isoclinic configuration $\overline{\mathbf{\Omega}}_i$ by the introduction of orthogonal rotation tensor $\widehat{\mathbf{R}}$before been transformed to the current configuration to get the Cauchy stress tensor at the end of f3dm93 subroutine.

Reference Theorems:

Before starting the implementation of the rotation tensor $\widehat{\mathbf{R}}$, a couple of points must be made. First of all, one must bear in mind that the proposed formulation insists on the existence of a unique orthogonal tensor $\widehat{\mathbf{R}}$ as well as a unique symmetric positive definite stretch tensor **U**for each invertible tensor **F**. In addition, as emphasised in (Brannon, R.M.,), the orthogonal tensor $\widehat{\mathbf{R}}$is considered a proper rotation if, and only if, $\det(\mathbf{F}) > 0$. Based on this discussion, the following theorem is adopted as a reference for a unique rotation tensor $\widehat{\mathbf{R}}$ implementation in the subroutine f3dm93 of Material Type 93.

Corresponding Author: M.K. Mohd Nor, Faculty of Mechanical Engineering and Manufacturing, Tun Hussein Onn University, Beg Berkunci 101 Parit Raja, Batu Pahat, 86400, Johor, Malaysia

- The deformation gradient$\mathbf{F}$is invertible
- The plastic stretch $\mathbf{U}$is symmetric and positive definite
- The rotation tensor $\hat{\mathbf{R}}$is orthogonalhence $\hat{\mathbf{R}}^{-1} = \hat{\mathbf{R}}^T$

Background of LLNL-DYNA3D Code:

This section briefly presents the background of this code. DYNA3D is basically an explicit finite element code that is used to study transient dynamic response. It is also known as a hydrocode, or an explicit three-dimensional finite element simulation code to solve finite deformation problems and inelastic materials that occur in a short time scale. This hydrocode is formulated based on the conservation of energy, mass and momentum equations. This code was initially developed at Lawrence Livermore National Laboratory (LLNL), and it has been widely used in LLNL and in many industries. In addition, the public DYNA3D code is maintained and developed by the Methods Development Group at LLNL.

DYNA3D is capable of formulating a variety of elements such as one dimensional truss, one dimensional beam elements, three-dimensional continuum elements and many more. Moreover, DYNA3D offers plenty of material models and equations of state, hence is able to represent a wide range of material behaviour, and also has the capability to model finite element analysis with a variety of modelling options. Equally, DYNA3D allows different bodies to interact as it contains several contact-impact algorithms.

DYNA3D was originally written with Fortran 77 language. Since the code has evolved rapidly, the programming of DYNA3D can now be optionally written with Fortran 90 language. In addition, it consists of over 80,000 FORTRAN lines of code, which can be divided into more than 800 subroutines. The implementation of the new orthogonal rotation tensor $\hat{\mathbf{R}}$is not easy to perform. Anyone who needs to modify the code must first learn the structure of the LLNL-DYNA3D code. Particularly, it is very useful to understand of the COMMON block, as well as the way that FORTRAN stores data in arrays when learning the DYNA3D code.

Implementation of Orthogonal Rotation Tensor $\hat{\boldsymbol{R}}$:

The implementation of the rotation tensor $\hat{\mathbf{R}}$into LLNL-DYNA3Dusing the deformation gradient tensor $\mathbf{F}$. This implementation is performed in the subroutine f3dm93 of the proposed constitutive model. It can be considered as one of the main parts of this subroutine. In addition, this tensor is calculated at the beginning of the subroutine f3dm93.

Referring to the given theorem, the first step of this tensor implementation is to calculate the inverse of the deformation gradient $\mathbf{F}$. This calculation immediately confirms that the deformation gradient $\mathbf{F}$ that passed into subroutine f3dm93 is correct and reliable for further calculation in this subroutine.

$$\mathbf{C} = \mathbf{F}^T \cdot \mathbf{F}. \quad (2)$$

Using the above equation, the 'helper' tensor, or more well-known as the Right Green tensor $\mathbf{C}$, is then calculated as a matrix uiu. Since tensor $\mathbf{C}$ is symmetric, only six of its components are calculated, named as $\mathrm{uiu}_{11}, \mathrm{uiu}_{22}, \mathrm{uiu}_{33}, \mathrm{uiu}_{12}, \mathrm{uiu}_{23}, \mathrm{uiu}_{13}$.

These components are passed to the subroutine jacob93 to identify the eigenvalues and the eigenvectors of this tensor. At the end of this subroutine, the eigenvalues and the eigenvectors of the selected matrix are calculated as outputs. In this case, the subroutine jacob93 calculates three eigenvalues $\mathrm{vals}(i)|\ i = 1,2,3$, and a $3x3$ eigenvectors matrix $\mathrm{vec}(i,j)|i,j = 1,2,3$, of a $3x3$ matrix uiu. By using these values, the plastic stretch tensor $\mathbf{U}$can be calculated using

$$\mathbf{U} = [\mathbf{A}]\begin{bmatrix} d_1 & 0 & 0 \\ 0 & d_2 & 0 \\ 0 & 0 & d_3 \end{bmatrix}[\mathbf{A}]^T \text{where } d_i \equiv +\sqrt{a_i} \quad (3)$$

As highlighted, the eigenvalues $d_i|i = 1,2,3$ are set to $+\sqrt{a_i}$. In addition, matrix $[\mathbf{A}]$ in Equation (3) contains the eigenvectors of $\mathbf{U}$. This formulation has been adopted in the implementation of the plastic stretch tensor $\mathbf{U}$of the proposed constitutive model, which is known as the diagonalisation of the matrix square root.

It is worth a reminder here that this algorithm is implemented to force the eigenvalues of tensor $\mathbf{C}$to be positive all of the time.Recalling the diagonalisation formulation in Equation (3), the value of plastic stretch tensor $\mathbf{U}$is also constrained to be positive by applying the absof the FORTRAN function. Once the plastic stretch tensor $\mathbf{U}$is obtained via the diagonalisation method, the corresponding inverse of this tensor is calculated to define the orthogonal rotation tensor $\hat{\mathbf{R}}$by using Equation (4).

$$\hat{\mathbf{R}} = \mathbf{F} \cdot \mathbf{U}^{-1}. \quad (4)$$

The diagonalisation method cannot guarantee the orthogonality of the rotation tensor $\hat{\mathbf{R}}$. Errors from a non-orthogonal rotation tensor $\hat{\mathbf{R}}$ will significantly affect the final result. The renormalisation method is then performed by rescaling the rotation tensor as follows

$$\hat{\mathbf{R}}^0 = \sqrt{\frac{3}{\mathrm{tr}(\hat{\mathbf{R}}^T\hat{\mathbf{R}})}}\hat{\mathbf{R}}. \quad (5)$$

Subsequently, again the subroutine jacob93 is used to calculate the eigenvalues and eigenvectors of tensor $\hat{\mathbf{R}}^0$. Eventually, Equation (6) is used to normalise and update the rotation tensor $\hat{\mathbf{R}}$ to the nearest orthonormal tensor.

$$\hat{\mathbf{R}}_{\mathrm{normalized}} = \frac{1}{2}\hat{\mathbf{R}}\left(3\mathbf{I} - \left(\hat{\mathbf{R}}\right)^T\hat{\mathbf{R}}\right). \quad (6)$$

Validation of the Proposed Algorithm:

To check and confirm the rotation tensor $\hat{\mathbf{R}}$that is calculated from the above algorithm is correct, the subroutine chkrot93 is called immediately after the renormalisation method. This subroutine is provided by Sandia National Laboratories in Brannon's work [3]. It is used to check whether the calculated rotation tensor $\widehat{\mathbf{R}}$ is a proper rotation tensor or not. The 'proper rotation' tensor $\widehat{\mathbf{R}}$ means that the rotation tensor must be orthogonal and the determinant is equal to +1. This subroutine requires only the candidate rotation tensor $\widehat{\mathbf{R}}$ in a matrix form as an input, and one value of output is generated then. The output variable is named IERR. In general, there are three different values of output that could possibly be obtained, depending on the examined rotation matrix $\widehat{\mathbf{R}}$:

- $\mathrm{IERR} = 0$, if the analysed matrix fulfils the proper rotation requirements.
- $\mathrm{IERR} = -1$, if the analysed matrix is orthogonal but has a negative determinant.
- $\mathrm{IERR} = \mathrm{ij}$, if the dot product between column i and column j is wrong. For instance, $\mathrm{IERR} = 33$ if column 3 of the rotation matrix is not normalised. In addition, $\mathrm{IERR} = 23$ if column 2 is not perpendicular to column 3.

The output generated from the subroutine chkrot93 is then passed to the subroutine f3dm93. The success of the rotation tensor $\widehat{\mathbf{R}}$ implementation means that the pull-back transformation upon the related variables from current $\mathbf{\Omega}_t$ to the isoclinic $\overline{\mathbf{\Omega}}_i$ configurations can be precisely performed.

Single Element Analysis:

To ensure the proposed algorihtm works properly in the DYNA3D when simulating the hardening behaviour of orthotropic materials, single element analysis of elastic-plastic model with linear hardening of Tantalumwas first conducted.The single element with the node numbering used to define boundary conditions is shown in Figure (1). In this model the principle directions of material orthotropy were aligned with the x, y, z axis of the global coordinate system. For brevity, only the tests performed in x direction are presented as presented in Table (1).

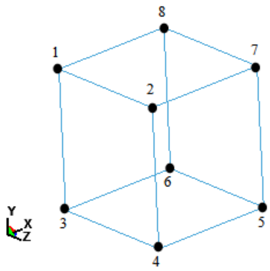

Fig. 1: Single Element Configuration.

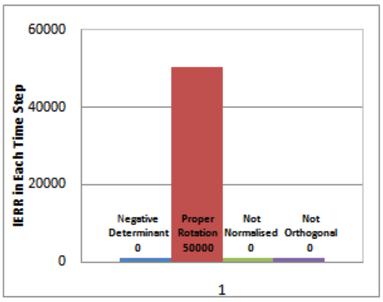

Fig. 2: chckrot93.f Output (IERR) for Uniaxial Stress Reversed Loading in X-Direction of Tantalum.

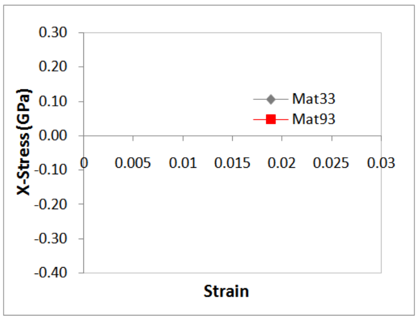

Fig. 3: Stress-Strain Curve of Proposed Formulation Mat93 vs. Reference Model Mat33 in X-Direction.

Table 1: Displacements boundary conditions for a Uniaxial Stress and Uniaxial Strain tests in the x direction.

Node Number	Displacement Boundary Condition	
	Uniaxial Stress	Uniaxial Strain
1	No constraints	Constrained y and z displacements
2	No constraints	Constrained y and z displacements
3	No constraints	Constrained y and z displacements
4	No constraints	Constrained y and z displacements
5	Constrained x, y and z displacements	Constrained x, y and z displacements
6	Constrained x displacement	Constrained x, y and z displacements
7	Constrained x displacement	Constrained x, y and z displacements
8	Constrained x displacement	Constrained x, y and z displacements

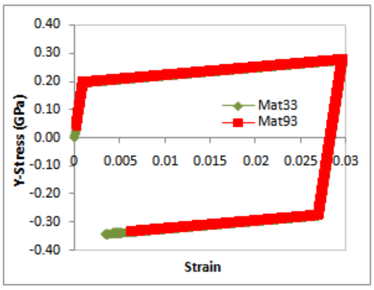

Fig. 4: Stress-Strain Curve of Proposed Formulation Mat93 vs. Reference Model Mat33 in Y-Direction.

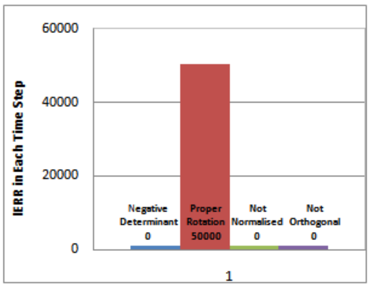

Fig. 5: chckrot93.f Output (IERR) for Uniaxial Stress Reversed Loading in Y-Direction of Tantalum.

Reversed loading in compression and tension was applied to the elements by prescribing displacement load curves to nodes 1, 2, 3 and 4. The equivalent tests were performed for the y and z directions. In order to speed up the comparison process, two solid elements with identical geometry, boundary conditions and loading were used in each simulation. In this model one element was assigned the new constitutive model (integrated in the isoclinic configuration) and the other a reference material model available in DYNA3D (Material Model 33). Material properties for this uniaxial reversed loading test can be found in. The density of tantalum was set to $16.64 \mathrm{gcm}^{-3}$.

To check, the output of the subroutine chkrot93 known as IERR that is passed to the subroutine f3dm93 in every time step was printed into the Fortran file and plotted into a graph. The establisehd constitutive model in DYNA3D used as a reference for comparison is the General Anisotropic Elastic-Plastic; Material Type 33. For the sake of brevity by setting the material axes AOPT 2 to $\mathbf{a} = 0\mathbf{a}_x + 0\mathbf{a}_y + 1\mathbf{a}_z$ and $\mathbf{d} = 0\mathbf{d}_x + 1\mathbf{d}_y + 0\mathbf{d}_z$, only the results obtained in x and y directions are presented:

Referring to Figures (2) to (5), it can be observed that the proposed constitutive model has successfully captured the elastic-plastic with hardening behaviours of Tantalum. The identical curves were provided by both material models within elastic-plastic regimes in each x and y directions. The Young's modulus, yield stress and the hardening slopes were identical in tension and compression. This good agreement was obtained by integrating the formulation precisely in the isoclinic configuration as the proposed algorithm calculates a proper rotation tensor in the selected material directions throughout the analysis.

Multiple Elements Analysis:

To ensure the book keeping of the proposed algorithm is efficientto model the behaviour of materials when impacted with shock loading at high impact velocity the validation process was continued with multiple elements analysis in this section against the Plate Impact test data of AA7010 published in [5]. Material properties for this test can be found in (Mohd Nor, M.K., 2012).

Figure (6) shows the configuration of the Plate Impact test simulation. It can be observed that the test consists of three parts of rectangular bars with $4x4$ elements. The first bar represents the PMMA block, while the second and third bars refer to the test specimen and flyer respectively. The mesh of this simulation was set to allow a 1D wave to propagate along the length of the bars when the impact happens. From this figure, it is noticed that symmetrical planes were adopted on all sides of the bars.

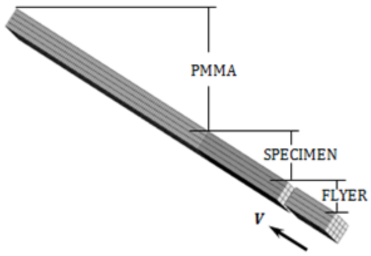

Fig. 6: Configuration of the Plate Impact test simulation.

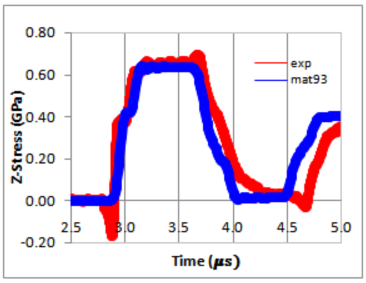

Fig. 7: Longitudinal stress (Z stress) comparison at 234ms^{-1} in longitudinal direction.

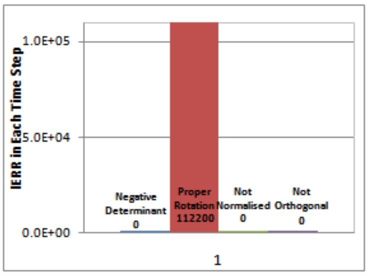

Fig. 8: IERR values at 234ms^{-1}in longitudinal direction.

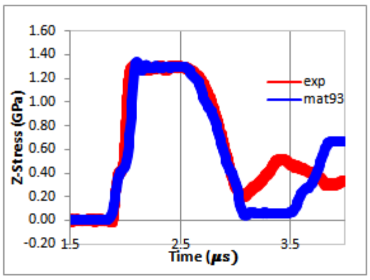

Fig. 9: Longitudinal stress (Z stress) comparison at 234ms^{-1} in longitudinal direction.

To ensure that no release wave was reflected from the back of the PMMA block into the test specimen, a non-reflecting boundary condition was applied to the back of this block (PMMA). In addition, the flyer, test specimen and PMMA bars were modelled with 25 elements, 75 elements and 100 elements respectively. They were modelled in parallel to the impact axis, while a contact interface was defined in between the flyer and the test specimen.

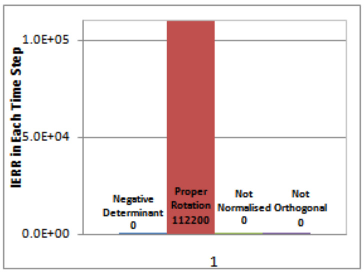

Fig. 10: IERR values at 450ms^{-1}in longitudinal direction.

To record the stress time histories of the impact, a time history block was defined in the elements at the top of PMMA bar. The same method as described in the preceding section was used to track the accuracy of integration in the isoclinic configuration. Two different impact velocities were performed in these analyses;234ms^{-1} and 450ms^{-1} as presented in the following figures.

Referring to the results shown in Figure (7) and Figure (9), it can be seen the elastic-plastic loading-unloading behaviours of the Al7010 were well captured by the proposed constitutive model, Material Type 93. A slope that was developed in the initial increment of the longitudinal stress represents the Hugoniot Elastic Limit (HEL). The width of the generated pulses in each analysis was reasonably agreed with the experimental test data. Furthermore, very close Hugoniot stress levels between the proposed constitutive model and the experimental data was also obtained by the newly implemented constitutive model that was preciselyintegrated in the isoclinic configuration since a proper rotation tensor was calculated by the new rotationtensor algorithm throughout the analysis as can be observed in Figures (8) and (10).

Conclusion:

A new rotation tensor algorithm was developed in the LLNL-DYNA3D code to correctly define the isoclinic configuration of constitutive model formulated for orthotropic materials in this paper. Several theorems were proved and applied to ensure a unique rotation tensor was successfully implemented into this code. Accordingly, a new subroutine was added to examine the accuracy of the newly implemented rotation tensor algorithm.

The uniaxial stress test of reversed loading and the Plate Impact test were conducted for a single and multiple elements analysis to validate the newly implemented algorithm respectively. The results obtained for both tests proved the integration were precisely performed in the isoclinic configuration throughout the analysis using the proposed algorithm and provide a satisfactory results with respect to the reference data.

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