ARL-TN-1180 ● Nov 2023

Consideration of Material Orientation for User-Defined Orthotropic Material Models in LS-DYNA

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ARL-TN-1180 ● NOV 2023

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REPORT DOCUMENTATION PAGE

1. REPORT DATE	2. REPORT TYPE	3. DATES COVERED START DATE	END DATE
November 2023	Technical Note	3/1/2022	9/29/2023

4. TITLE AND SUBTITLE
Consideration of Material Orientation for User-Defined Orthotropic Material Models in LS-DYNA

5a. CONTRACT NUMBER	5b. GRANT NUMBER	5c. PROGRAM ELEMENT NUMBER
5d. PROJECT NUMBER	**5e. TASK NUMBER**	**5f. WORK UNIT NUMBER**

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8. PERFORMING ORGANIZATION REPORT NUMBER
ARL-TN-1180

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)	11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
DISTRIBUTION STATEMENT A. Approved for public release: distribution unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT
Simulations involving materials with orientation dependence (e.g., composites) must consider the change in material orientation as the component is rotated or deformed. Finite element simulation tools provide two basic frameworks to accommodate the orientation change. One method is to evaluate the material behavior in its current orientation in the global coordinate system. The second method evaluates the constitutive model in the material frame. LS-DYNA typically evaluates anisotropic constitutive models in the latter. This requires evolving the material reference frame and mapping strain rate and prior stress from the global frame to the material frame. This report explores how LS-DYNA handles this evolution and mapping for user-defined material models in explicit simulations. It also provides evaluations of options for controlling the mapping along with providing potential methods for further controlling the mapping.

15. SUBJECT TERMS
Terminal Effects, LS-DYNA, constitutive modeling, anisotropic materials, material reference frame, material orientation

16. SECURITY CLASSIFICATION OF: a. REPORT	b. ABSTRACT	C. THIS PAGE	17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UU	21

19a. NAME OF RESPONSIBLE PERSON	19b. PHONE NUMBER *(Include area code)*
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STANDARD FORM 298 (REV. 5/2020)
Prescribed by ANSI Std. Z39.18

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Acknowledgments

I would like to thank Dr Richard Becker of DEVCOM Army Research Laboratory for providing guidance and his insightful comments throughout this investigation.

1. Introduction and Background

Simulations involving materials with orientation dependence, such as composites or metals and polymers with processing direction dependence, must consider the change in material orientation as the component is rotated or deformed. The orientation is tied to variables or parameters managed by the material constitutive model. Finite element simulation tools provide two basic frameworks to accommodate the orientation change. One is to evaluate the material behavior in its current orientation in the global coordinate system. This involves evolving the material orientation with every time step using internal variables associated with the material orientation. The other method assumes that the material preferred directions evolve with the material rotation. In this method, the constitutive model is evaluated in the material reference frame where the material orientations are assumed to be fixed, obviating the need to update the material directions for component rotation. The evolution of this material reference frame in LS-DYNA is the subject of this report.

The material rotation is clear and unambiguous for rigid body rotations. When rotation and deformation occur concurrently, particularly shear deformation, the rotation of a proper material reference frame can also depend on the material's constitutive behavior. This constitutive model dependence is often neglected as being small, and the material reference frame is commonly assumed to follow the rotation of the RU polar decomposition of the deformation gradient, where R is the rotation and U is the deformation. To integrate material models in the material frame, the strain rate and prior stresses are mapped into the material frame using the transpose of the rotation. These are used to update the stress and history variables in the material frame. The stress is then mapped back to the global coordinate system for use in the finite element equations. In LS-DYNA, however, the material reference frame is assumed to evolve with vectors associated with the Lagrangian finite elements rather than the polar decomposition of the deformation gradient. This report explores how LS-DYNA handles these transformations and some of the effects that various LS-DYNA options have.

This study was completed by examining the transformation tensor used by LS-DYNA when a user-defined material subroutine was used. A simple linear isotropic elastic material model was used; however, when defining the material model, IORTHO was set to 1 indicating the material is orthotropic. (IHYPER was also set to 1 to provide the deformation gradient to the user-defined subroutine.) This flag prompts LS-DYNA to assemble a transformation tensor and to map the strain rate and prior stress to the material frame (from the global frame).

When LS-DYNA assembles this transformation tensor, it accounts for a two-step transformation: first, from the global coordinate system to the element coordinate system, and then from the element coordinate system to the material coordinate system. The transformation between the element coordinate system to the material coordinate system is set and fixed at the beginning of the simulation. Rotation of the element coordinate system during the simulation leads to the updated material coordinate system orientation.

One LS-DYNA option that affects how the element orientation updates is the invariant node numbering (INN) option in the CONTROL_ACCURACY card. In LS-DYNA, by default for solid elements in explicit simulations (INN=1), the element system is defined as the x-direction from node 1 to node 2; the y-direction orthogonal to x and in the plane defined by node 1, node 2, and node 4. Setting INN=3 makes the local element system insensitive to the order of the nodes defined by the element connectivity. In this report, both INN set to off (i.e., INN=1) and INN=3 where examined.

In addition to the previously described options, Livermore Software Technology Corporation, an ANSYS company,[1] suggested some additional methods for controlling the mapping to and from the material frame that could be used for greater control over the mapping procedure. These will be in Section 4.

2. Methodology

Three test cases were used in this study to examine the transformation tensor that LS-DYNA uses to map the strain rate and prior stress to the material frame before passing them to the user-defined material subroutine. Version R10.1 of LS-DYNA was used for this study.[2] Nodal displacements were prescribed in the simulations to achieve the following conditions: pure rotation, simple shear, and extension. All the nodal motions in these simulations were within the X-Z plane. In all simulations, the initial material coordinate system for each element was prescribed to be aligned with the global coordinate system (i.e., a-axis aligned with x-axis; b-axis aligned with y-axis; and c-axis aligned with z-axis) (See Fig. 1 for initial orientation.) Due to these two facts, the transformation tensor(Z) used by LS-DYNA represents a single in-plane rotation from the initial (global) material coordinate system to the final material coordinate system orientation. Throughout the rest of analysis, the arcsin(Z^T_{13}), which represents the rotation about the y-axis, will be presented for comparison against analytical solutions for each test. To have access to this information, several print statements were inserted into the LS-DYNA subroutine urmathn() in the file dyn21.f, and the program was recompiled. The print statements allowed the code to output the transformation tensor and the strain increments during each step of the simulation for each element in the simulation.

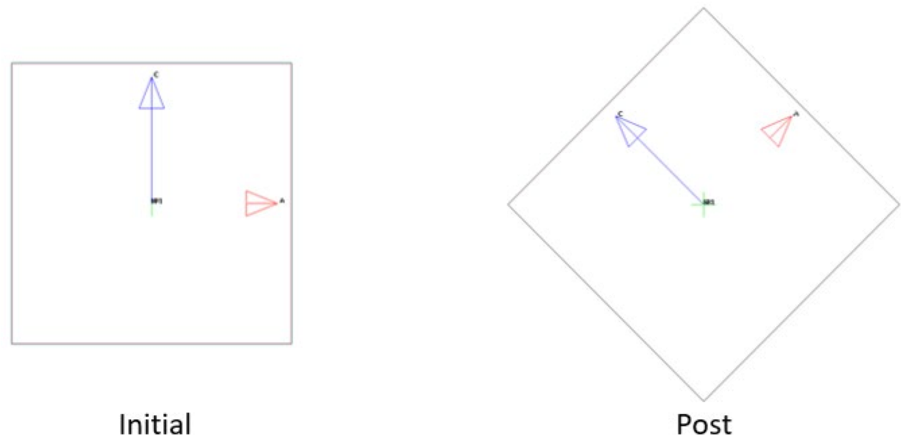

Fig. 1 Initial and final configuration of the element along with material coordinate system for the pure rotation test case. a-axis (red) initially aligned with global x-axis. b-axis (green) initially aligned with global y-axis (into plane). c-axis (blue) initially aligned with global z-axis.

The rotation from the RU polar decomposition of the deformation gradient tensor is used in several computational solid mechanics codes to map strain rate and prior stress from the global to the material frame. The analytical solution used for comparison in this study will be arcsin(R_13). If the rotation tensor from the RU polar decomposition of the deformation gradient was being used to go between the material and current frame, the resulting transformation tensor would be its transpose, or more commonly R $= Q^T = Z^T$. Thus, the rotation described by arcsin(Z^T_{13}) will be compared to arcsin(R_{13}) in this study.

3. Results

3.1 Test Case 1: Pure Rotation

The first case examined is a pure rotation. A single cubic element is rotated counterclockwise 45° (with the given coordinate system this equates to a negative 45° rotation of the element about the global y-axis, which is into the plane). The initial and final orientations of the element are shown in Fig. 1. The simulation was run with both INN=1 and 3. The rotation that LS-DYNA used to map the strain rate and prior stress throughout the simulation are shown in Fig. 2 for both INN=1 and 3. Based on the results, the INN option does not change the rotation LS-DYNA uses for a case of pure rotation. In addition, LS-DYNA's internal transformation tensor from global to material coordinate systems matches the analytical solution (see Eq. 1) for the rotation imposed on the element.

$$F = R \cdot U = \begin{bmatrix} \cos(\theta) & 0 & \sin(\theta) \\ 0 & 1 & 0 \\ -\sin(\theta) & 0 & \cos(\theta) \end{bmatrix} = \begin{bmatrix} \cos(\theta) & 0 & \sin(\theta) \\ 0 & 1 & 0 \\ -\sin(\theta) & 0 & \cos(\theta) \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (1)$$

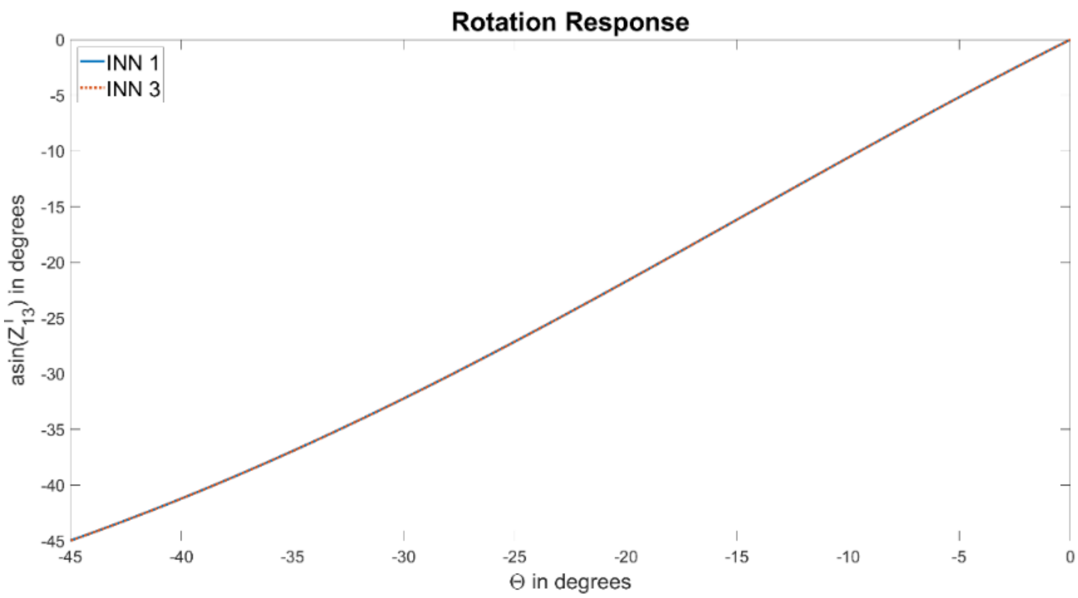

Fig. 2 Rotation of material coordinate system about the y-axis for the pure rotation test

3.2 Test Case 2: Simple Shear

The second case examined was simple shear. Three sets of simulations were run to examine the rotation that LS-DYNA uses to map the stresses and strains and the effects that the INN option has on them. First, a set of three different shaped single element meshes were run under simple shear loading. Then another single element simulation was run with the shearing directed in the vertical direction. The final set of simulations run under a simple shear condition was a set of four-element meshes of a cube. For all these simulations, prescribed nodal motions were applied such that a simple shear deformation gradient was applied to the material model.

Equation 2 describes the deformation gradient simulated with gamma (γ) going from 0 to 1 in the simulations. Equation 2 shows the analytical solution for the rotation tensor that the LS-DYNA results are compared against. Again, the simulations were run with both INN=1 and 3.

$$F = R \cdot U = \begin{bmatrix} 1 & 0 & \gamma \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \frac{1}{\sqrt{1+\frac{\gamma^2}{4}}} \begin{bmatrix} 1 & 0 & \frac{\gamma}{2} \\ 0 & 1 & 0 \\ -\frac{\gamma}{2} & 0 & 1 \end{bmatrix} \cdot \frac{1}{\sqrt{1+\frac{\gamma^2}{4}}} \begin{bmatrix} 1 & 0 & \frac{\gamma}{2} \\ 0 & 1 & 0 \\ \frac{\gamma}{2} & 0 & 1+\frac{\gamma^2}{2} \end{bmatrix} \quad (2)$$

3.2.1 Test Case: Simple Shear—Single Element

The first simple shear test consisted of three single element meshes: one cubic element and two pre-deformed right rhombic prisms with different starting orientations (Fig. 3). All three simulations start with the material orientation in the same direction. For the analytical comparison, this corresponds to an undeformed material at the start of the simulation. The results for the three meshes with INN=3 can be seen in Fig. 4. With the invariant node numbering on, each material orientation is rotated during the simulations. However, this occurs at different rates for each starting element shape. The only result that agrees well with the analytical solution is for the standard cubic element (Mesh 1), and that is only at smaller strains. The results for the cubic element start to diverge at $\gamma \sim 0.26$.

The results for this test with INN=1 was omitted here because they all correspond to zero rotation to the material orientation throughout the simulated shearing. This is due to the nodal numbering used when the mesh was defined. The nodes determining the element orientation do not change relevant position with this direction of loading, so there is no corresponding rotation to the material coordinate system.

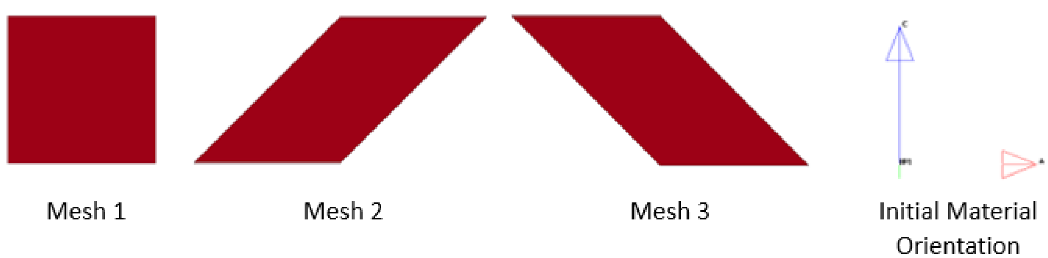

Fig. 3 Initial mesh configurations for the single element simple shear test. a-axis (red) initially aligned with global x-axis. b-axis (green) initially aligned with global y-axis (into plane). c-axis (blue) initially aligned with global z-axis.

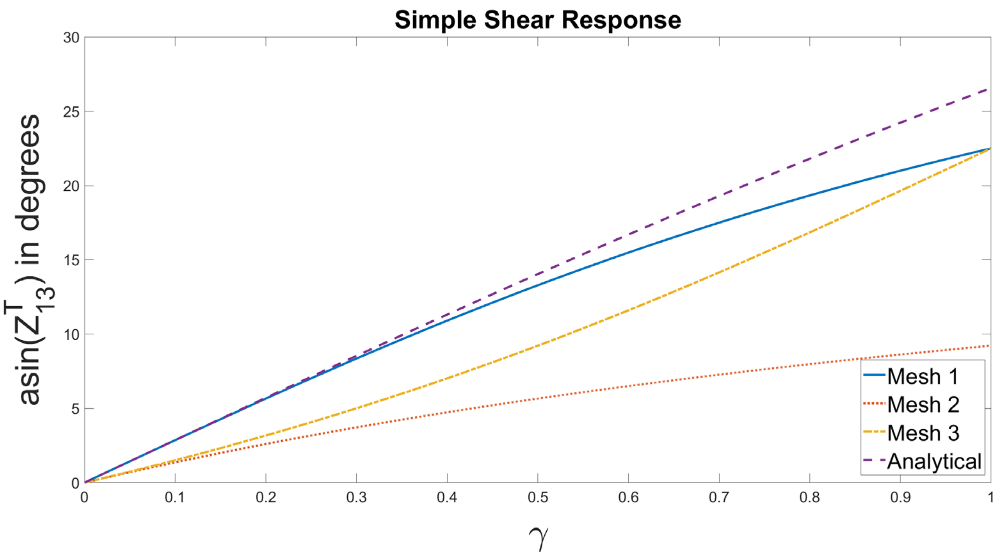

Fig. 4 Rotation of material coordinate system about the y-axis for the single element simple shear test with INN=3

3.2.2 Test Case: Simple Shear—Differing Shear Direction

The second simple shear test consisted of a single element sheared in two separate directions (either horizontally or vertically). The element shape and material orientations pre- and post-shearing are shown in Fig. 5. These two loading scenarios would analytically result in the same final material orientation. Without invariant node numbering, the two loading conditions result in two distinct final material orientations. For horizontal shearing, there is no rotation of the material coordinate system. For the vertical shearing, the rotation follows the motion of the bottom face of the cube. Again, this disparity is due to the initial node numbering used in the mesh generation and how element orientation is determined by LS-DYNA. With the invariant node numbering turned on, the results for the two shearing directions are the same; however, the results do not match the analytical solution. The rotation is the same as the cubic element (Mesh 1) from the previous study.

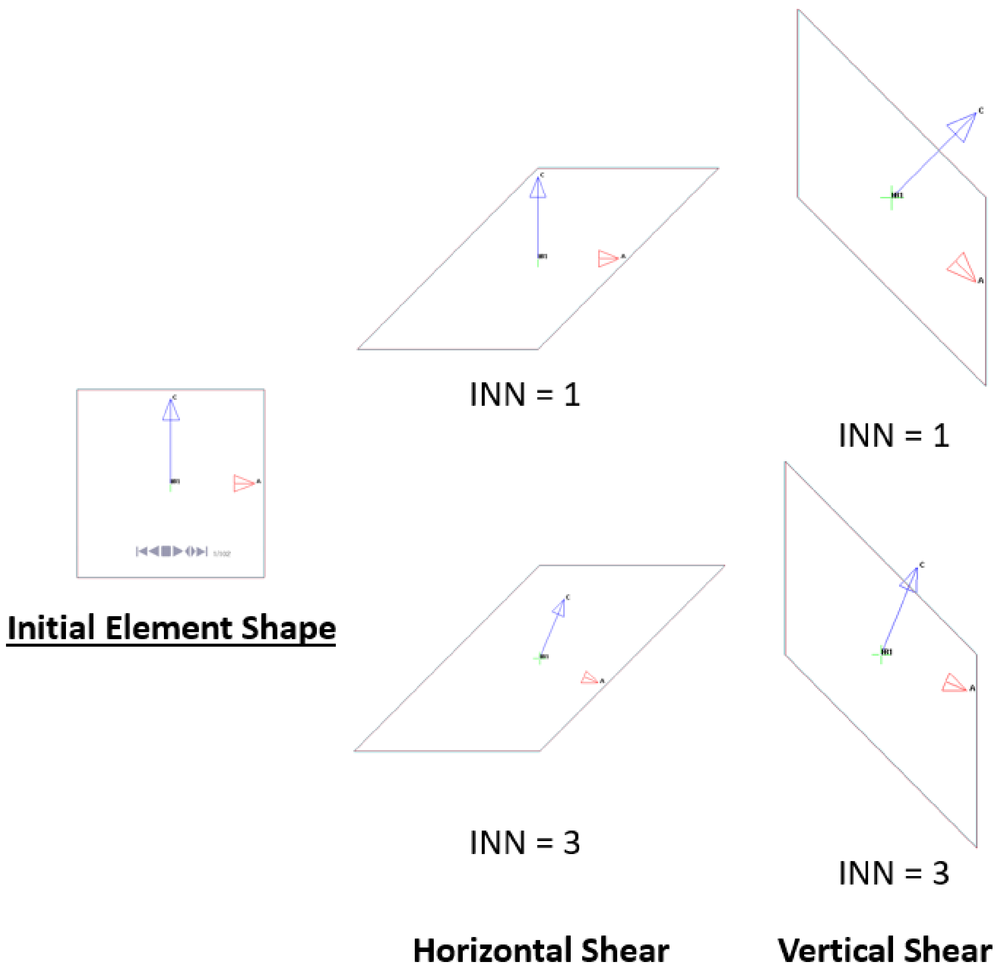

Fig. 5 Comparison of the rotation of the material coordinate system to differing simple shear direction and INN options. Note: for explicit simulations, INN=1 is the default option. a-axis (red) initially aligned with global x-axis. b-axis (green) initially aligned with global y-axis (into plane). c-axis (blue) initially aligned with global z-axis.

3.2.3 Test Case: Simple Shear—Multiple Element

The third simple shear test consisted of three four-element cubic meshes with the same initial material orientation but differing initial element shapes (Fig. 6). Analytically, all elements in each case have the same material orientation throughout the deformation; however, that is not observed in most of the simulations (see Figs. 7 and 8). Mesh 2, which had uniform rectangular prism elements and consistent material orientation, is the exception. The results for INN=1 and 3 are different with the results for INN=3 being much closer to the analytical solution.

The results for the simulations without invariant node numbering tend to have more divergence from element-to-element (~40° maximum divergence) in the same mesh in comparison to the simulations with invariant node numbering (~10°

maximum divergence). Furthermore, the results for the simulations with invariant node numbering tend to be closer to the analytical solution when compared to simulations without invariant node numbering.

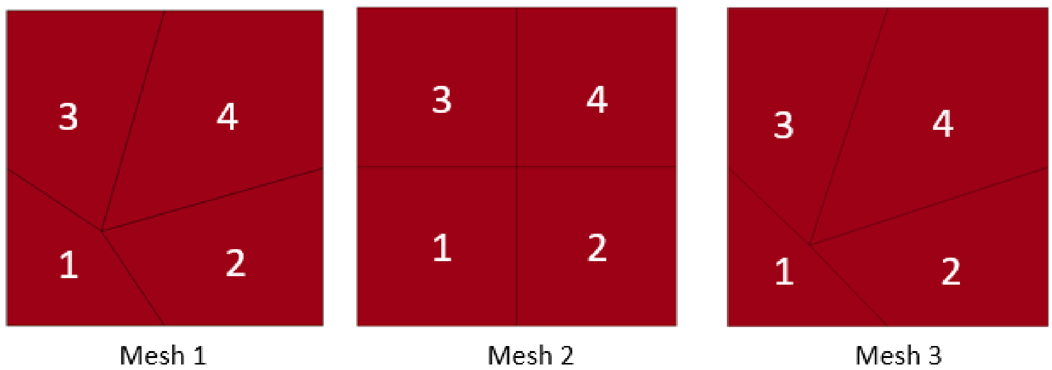

Fig. 6 Initial mesh configurations for the multi-element simple shear test. Element numbers are shown in white for each mesh.

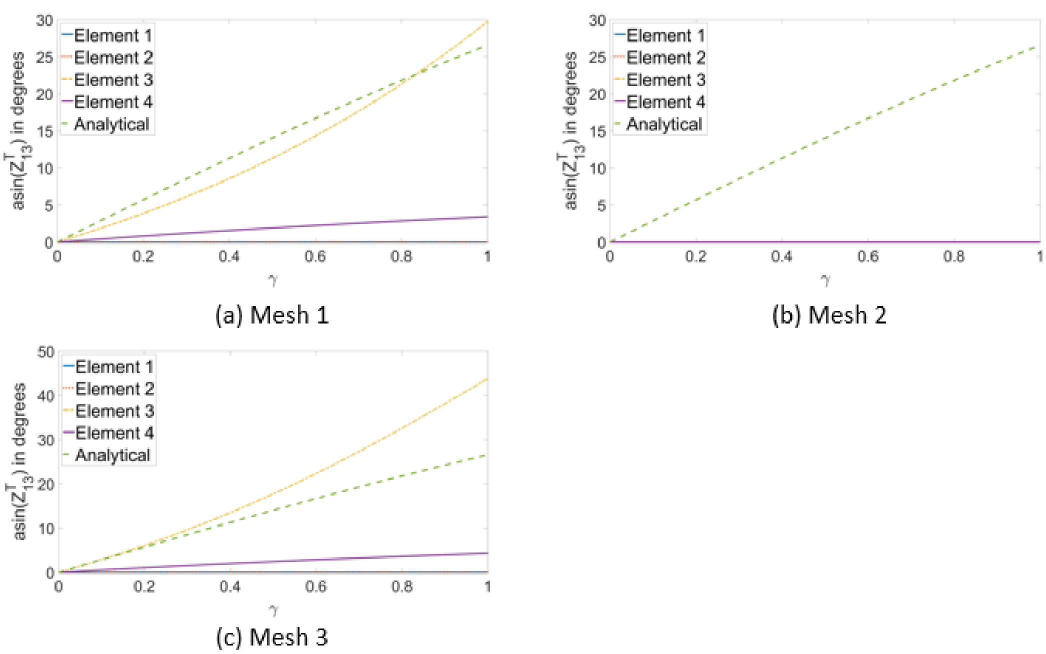

Fig. 7 Rotation of material coordinate system about the y-axis for the multi-element simple shear test with INN=1. (a) Mesh 1 results, (b) Mesh 2 results, and (c) Mesh 3 results.

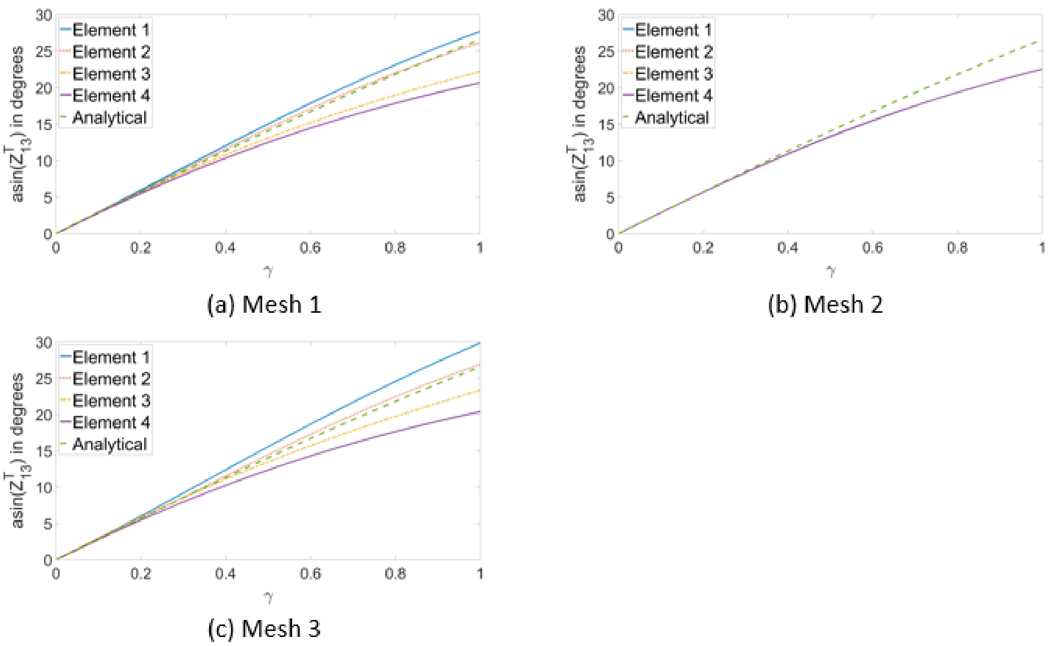

Fig. 8 Rotation of material coordinate system about the y-axis for the multi-element simple shear test with INN=3. (a) Mesh 1 results, (b) Mesh 2 results, and (c) Mesh 3 results.

3.3. Test Case 3: Extension

The third test case examined in this study was that of extension (in the vertical direction/along the z-axis) of a cube with four elements. The three different meshes examined for this case are shown in Fig. 9. The deformation gradient applied to the mesh is defined by Eq. 3 with λ going from 1 to 2. The analytical solution for the rotation tensor (R) that the LS-DYNA results are compared against is also shown in Eq. 3. There should be no rotation from the global coordinate system to the material coordinate system in these simulations. Again, the simulations were run with invariant node numbering on and off.

$$F = R \cdot U = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \lambda \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \lambda \end{bmatrix} \tag{3}$$

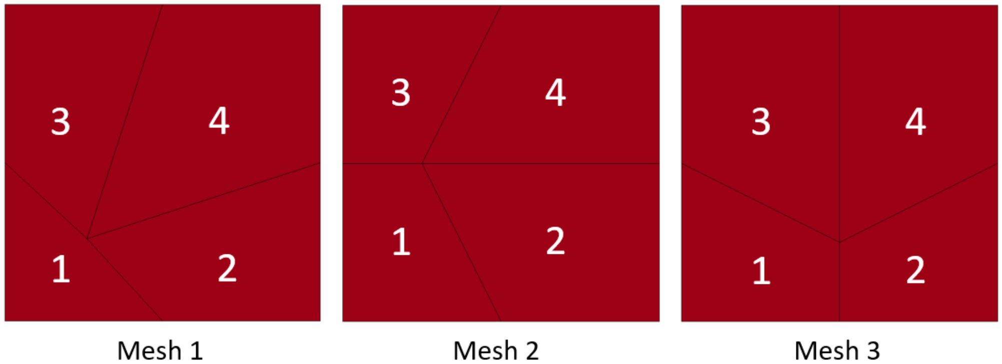

Fig. 9 Initial mesh configurations for the multi-element extension test. Element numbers are shown in white for each mesh.

The results for these simulations are shown in Figs. 10 and 11. In all cases except Mesh 2 with INN=1, there are rotations present from the global to the material coordinate systems. For Mesh 2 with INN=1, the lack of rotation is purely a function of node numbering defining the elements. The edges of the elements determining the material coordinate system orientation happened to align with the deformation similar to the results for Mesh 2 of the multi-element simple shear test. Reordering the node numbers for Mesh 2 would result in a rotation between the global and material frame during the simulation.

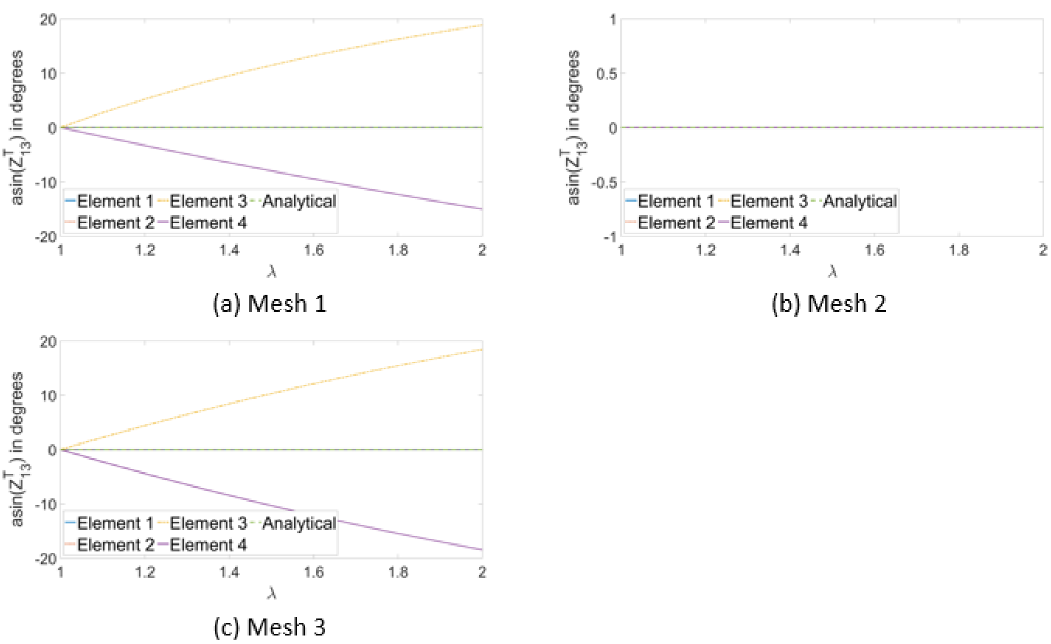

Fig. 10 Rotation of material coordinate system about the y-axis for the multi-element extension test with INN=1. (a) Mesh 1 results, (b) Mesh 2 results, and (c) Mesh 3 results.

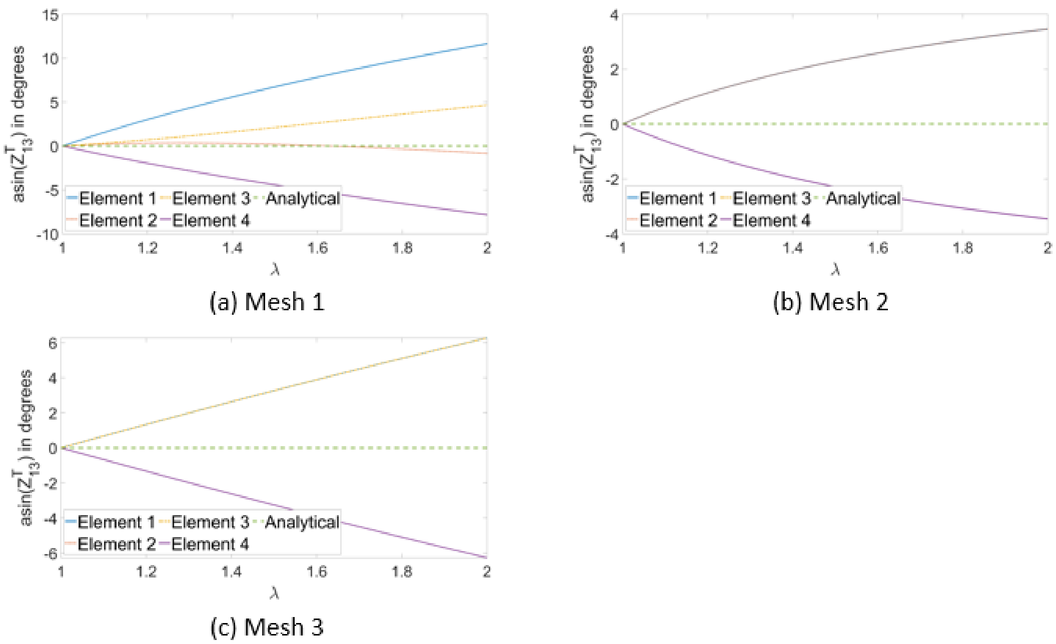

Fig. 11 Rotation of material coordinate system about the y-axis for the multi-element extension test with INN=3. (a) Mesh 1 results, (b) Mesh 2 results, and (c) Mesh 3 results.

For simulations with INN=3, all meshes resulted in rotations from the global to material coordinate systems, which is a divergence from the analytical rotation. For this test case Meshes 2 and 3 are symmetric, and the rotations observed correspondingly fall into one of two rotations. The asymmetry in Mesh 1 results in a unique rotation for each element. However, for these meshes with INN=1, either one or three rotation angles were observed.

Once again, the simulation results without invariant node numbering tend to have more divergence from element-to-element (~40° maximum divergence) in the same mesh in comparison to the simulations with invariant node numbering (~20° maximum divergence). The exception to this is Mesh 2, which was discussed previously.

4. Conclusion

The transformation between the global to material frame in LS-DYNA (version R10.1) for user-defined orthotropic material models was explored along with the effects of several LS-DYNA options. While the analyses shown here were completed in LS-DYNA version R10.1, the divergences in the rotation in the material frame was still verified to exist in version R14.0. The transformation was compared to a transformation (rotation based on a polar decomposition of the deformation gradient) commonly used in other solid mechanics codes.

Based on the results shown, several conclusions can be drawn about the transformation used by LS-DYNA for user-defined orthotropic (IORTHO=1) material models. First, the transformation is based on a combination of element rotation and deformation, not the deformation gradient applied to the element. Second, applying the same deformation gradient to elements of differing shapes tends to result in different material coordinate system orientations. However, this can be affected by specific node numbering in combination with specific loading conditions along with the choice of INN=1 or 3. Third, in most cases, element-to-element divergence in the material frame orientation is lessened and a closer match to the transformation from the analytical solutions is observed by setting INN=3. This option also increases consistency of the responses under different loading directions.

In addition to understanding the standard behavior of the transformation behavior as just described, it could be useful to have user-defined material models that would yield the same results between several solid mechanics codes for comparison. Per a discussion with Livermore Software Technology Corporation, an ANSYS company,[1] there are several ways that using the rotation from the polar decomposition of the deformation gradient could be implemented to rotate from the global to the desired material frame. The first option would be to have IORTHO off and internally within the user-defined material model handle the rotations of the stresses and strains based on the polar decomposition of the deformation gradient. The second option is to have IORTHO on, but replace the calculation for the transformation from the global to material frame in the urmathn() subroutine in dyna21.f. Following either of these procedures would allow for comparison between other solid mechanics codes that handle this rotation internally.

Furthermore, implementing one of these two solutions for orthotropic user-defined materials would ensure that elements (even if initially distorted) experiencing the same deformation gradients would have the same transformation between the global to material frames throughout the simulation.

5. References

1. Technical support. Livermore Software Technology Corporation, an ANSYS company. Email communication, 2022 Mar 26.

2. LS-DYNA. LS-DYNA keyword user's manual volume I, II, III. Version R10.1. Livermore Software Technology Corporation; 2018 Feb.

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