LAWRENCE LIVERMORE NATIONAL LABORATORY

LLNL-TR-851544

Verification Testing of Body Forces due to a Prescribed Angular Velocity in DYNA3D/Paradyn

M. J. Zoller

July 14, 2023

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Verification/Regression Testing of Body Forces due to a Prescribed Angular Velocity in DYNA3D/Paradyn

Miklos Johann Zoller
Methods Development Group
Computational Engineering Division

July 6, 2023

Executive Summary

This report documents the verification testing and regression testing done on a new feature in DYNA3D/Paradyn, which allows users to prescribe body force loads based upon an angular velocity. This feature is unique in that the direction of the angular velocity vector follows the unit vector formed by two coordinate points associated with two nodes or the average coordinates of two separate small collection of nodes. The angular velocity direction will follow the directional vector defined by these nodes while the angular velocity magnitude is defined by a load curve. A simple single element verification test was performed to determine the correct implementation of this feature, and two separate regression tests were added to the DYNA3D Software Quality Assurance test suite. The nodal positions, velocities, and accelerations from the solution of the single element verification test compare well to analytically derived values of those nodal quantities. The regression tests serve as good examples of this new feature's use case and were consequently added to the SQA test suite to ensure that further modifications of the DYNA3D source code do not unintentionally change the generated baseline answers.

1 Introduction

DYNA3D previously had the ability to prescribe a body force load due to an angular velocity except the angular velocity direction was always fixed in space along the x, y, and z axes according to a user's input. This provided a sufficient capability if the system experienced little rotation as the simulation progressed. If moderate to large rotations occurred, then the body force loads computed could be physically inaccurate and could perturb the system and cause chaotic and nonphysical motion. Therefore, it was desired that a follower type of body force could be defined, where the angular velocity direction is updated as the simulation solution progresses. The unit direction of the angular velocity would be continuously updated based upon the coordinate values of two nodes or the average coordinate values of two separate small collections of nodes. This new feature would help mitigate any instability formed by systems undergoing moderate to large rotations when body force loads due to prescribed angular velocities are applied.

The new feature decomposes the angular velocity $\boldsymbol{\omega}$ into a magnitude and unit direction, $\boldsymbol{\omega} = \hat{\omega}(t)\boldsymbol{\omega}_n$, where $\|\boldsymbol{\omega}_n\| = 1$ and $\hat{\omega}$ is a function of time. The magnitude of the angular velocity $\hat{\omega}$ is given by a user defined load curve. The direction is defined according to the expression,

$$\boldsymbol{\omega}_n = \|\bar{\mathbf{x}}_2 - \bar{\mathbf{x}}_1\| , \tag{1}$$

where $\bar{\mathbf{x}}_2$ and $\bar{\mathbf{x}}_1$ are the coordinates of two user specified node labels or the average coordinates of two distinct collections of nodes. There are two ways of specifying $\bar{\mathbf{x}}_1$ and $\bar{\mathbf{x}}_2$ to allow for generality in defining the base and tip of a directional unit vector.

The first way is that a user can specify that the angular velocity follow the unit vector formed by 2 specific node labels. For example, a user can request that the angular velocity be defined about the node labels 5 and 14, where the current nodal positions are given as $(0.5, 0.25, 0.75)$ and $(1.0, -0.25, 1.25)$, respectively. This would yield $\boldsymbol{\omega}_n = \|(1.0 - 0.5, -0.25 - 0.25, 1.25 - 0.75)\| = (\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$. This option is enacted in DYNA3D through the keyword `node_labels` and is further explained in Zywicz et al. [2022].

Another way is that a user chooses of a small collection of node labels defining the average coordinates for the base and tip of the direction vector. The keyword `node1_labels` would define the node labels corresponding to the base of the vector, and the keyword `node2_labels` would define the node labels corresponding to the tip of the vector. Suppose a user specifies that node labels 1 and 3 correspond to the base of the vector (i.e. `node1_labels`) and that node labels 9 and 12 correspond to the tip of the vector (i.e. `node2_labels`). Then, $\bar{\mathbf{x}}_1 = \frac{1}{2}(\mathbf{x}_1 + \mathbf{x}_3)$ and $\bar{\mathbf{x}}_2 = \frac{1}{2}(\mathbf{x}_9 + \mathbf{x}_{12})$, where $\mathbf{x}_i$ is the position vector of the i^{th} node, and the expression above for $\boldsymbol{\omega}_n$ is used to determine the unit direction of the angular velocity.

Ultimately, once an angular velocity $\boldsymbol{\omega}$ is fully defined, then a body force density at a point $\mathbf{x}$ is determined according to the relation,

$$\mathbf{b} = \rho\left(\boldsymbol{\omega} \times \boldsymbol{\omega} \times \mathbf{r}\right) , \tag{2}$$

where ρ is the material density and $\mathbf{r} = \mathbf{x} - \mathbf{p}$ is the relative nodal position vector about a user specified point $\mathbf{p}$. Given a particular nodal position $\mathbf{x}_i$, the body force $\mathbf{b}$ is computed according to the expression above and added to the external nodal force array $\mathbf{f}_{ext}$. The remaining two sections in this report document the testing done to verify the correct implementation of Eq. (2) in DYNA3D.

2 Verification Test

A single 8-node hexahedral element is used to verify the expected results of an applied body force load given a prescribed angular velocity. The single element test is illustrated in Figure

1, where the angular velocity direction is defined according to nodes 1 and 5 yielding the vector $\boldsymbol{\omega}$ in the figure. The magnitude of the angular velocity is constant in time and is equal to 1000.0 rad/s. The center of rotation coordinates are $\mathbf{p} = (0, 0, 0)$ and coincides with the nodal coordinates of node 1. The length of each side of the element is equal to 1.0 to yield a unit cube. The element uses a hypoelastic isotropic material model, where $E = 10^{-7}$, $\nu = 0$, and $\rho = 1$. The magnitude of the Young's modulus E was chosen to be sufficiently small to minimize numerical contributions to the nodal accelerations emanating from the internal force calculations. Note that the internal forces are used to determine the total nodal accelerations in the system and are inherent in solving the equations of motion for the element. In this test, the element only computes an external force based upon the global body force load described above, and the DYNA3D simulation is run for a total of 10 cycles for $t \in [0, 1.0 \times 10^{-4}]$ with a fixed $\Delta t = 10^{-5}$. Lastly, nodes 1 and 5 are permanently fixed in space in the x and y directions but are free to move in the z direction. Due to the symmetric nature of the simulation and given $\nu = 0$, the element will expand and contract along the xy plane and should not exhibit any movement along the z axis. This is evident in the results, as the DYNA3D values for a_z, v_z, and d_z are zero for all nodes at each discrete point in time. Additionally, the symmetry of the problem allows one to study only either the x or y motion of a particular node. For this reason, this report only documents the motion along the x direction of node 8 in this verification test.

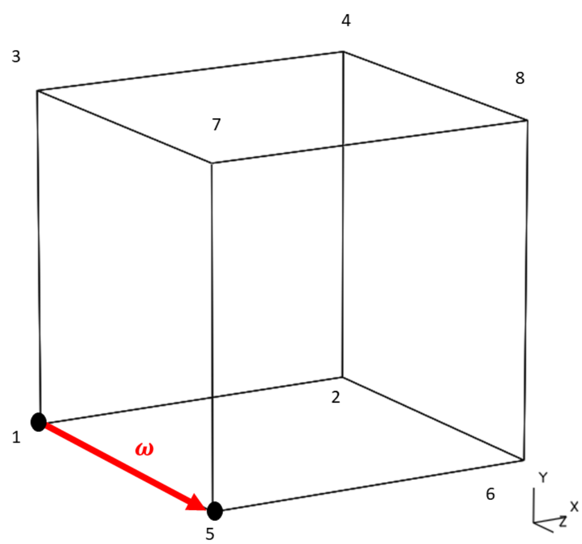


Figure 1: Single element verification test with angular velocity vector defined about nodes 1 and 5 denoting the base and tip of the angular velocity direction, respectively.

Given the body force load defined above, this verification test compares the outputted DYNA3D nodal displacements, velocities, and accelerations of node 8 with those derived from an analytical solution using the explicit time integration scheme described below. A relative error value is computed at each time step and is defined according to the relation

$$\epsilon = \left| \frac{x_{dyna} - x_{analytical}}{x_{analytical}} \right|, \tag{3}$$

where x_{dyna} is the outputted DYNA3D value of the quantity in question and $x_{analytical}$ is its value determined by the analytical explicit time integration scheme.

The explicit time integration scheme is given in Belytschko et al. [2014] and is outlined as follows:

1. Initialization of initial conditions: set $\mathbf{d}_0$, $\mathbf{v}_0$, and $\mathbf{a}_0$
2. Determine the body force using Eq. (2) and divide by material density ρ to determine acceleration of each node $\mathbf{a}_n$ at t_n
3. Update time: $t_{n+1} = t_n + \Delta t$
4. Compute first partial update to nodal velocities: $\mathbf{v}_{n+1/2} = \mathbf{v}_n + \frac{\Delta t}{2}\mathbf{a}_n$
5. Update nodal displacements: $\mathbf{d}_{n+1} = \mathbf{d}_n + \Delta t \cdot \mathbf{v}_{n+1/2}$
6. Determine the body force using Eq. (2) and divide by material density ρ to determine acceleration of each node $\mathbf{a}_{n+1}$ at t_{n+1}
7. Compute second partial update to nodal velocities: $\mathbf{v}_{n+1} = \mathbf{v}_{n+1/2} + \frac{\Delta t}{2}\mathbf{a}_{n+1}$
8. Update counter $(n \to n+1)$ and go to 3.

The integration scheme above is used for node 8, and the relative error results for the accelerations, velocities, and displacements are shown in Tables 1, 2, and 3, respectively. Note that the resulting algorithm above neglects the contribution of the stress divergence term (i.e. internal forces due to the material constitutive law) in computing the nodal accelerations and is an inherent difference between the DYNA3D output and the analytical solution presented in this section. To remedy this, the chosen value of E was chosen to be sufficiently small enough in comparison to the applied body force loads. Additionally, the integration scheme does not consider changes in the element volume and integration over the element domain, which is another inherent difference and source of error in the derived analytical solution. Evident by the increasing magnitude of the relative errors as time progressed in the simulation, these two sources of error should have been included to yield a more accurate analytical solution. Nevertheless, the relative error values are on the order of numerical precision for the first time step ($t = 1.0 \times 10^{-5}$) for the x component of the acceleration, velocity, and displacement of node 8 and deems that the DYNA3D feature is implemented correctly . This is also apparent in Figures 2 and 3, where the x and y velocity and displacement components of the DYNA3D solution and analytical solution match extremely well. Ultimately, the resulting divergence of the analytical and DYNA3D values of the x and y accelerations can be contributed to the neglection of the stress divergence term and failure to properly integrate over the element domain in the analytical derivation. However, this does not present an error in the feature's implementation.

Time: t	X **Acceleration**	**Analytical Value**	**Relative Error**: ϵ
0.0e+00	1.000000000000e+06	1.000000000000e+06	0.000000000000e+00
1.0e-05	1.000050000000e+06	1.000050000000e+06	1.164095013519e-16
2.0e-05	1.000200005000e+06	1.000250005000e+06	4.998750287446e-05
3.0e-05	1.000450030001e+06	1.000700040000e+06	2.498351054326e-04
4.0e-05	1.000800100004e+06	1.001500175005e+06	6.990263396570e-04
5.0e-05	1.001250250018e+06	1.002750560033e+06	1.496194641818e-03
6.0e-05	1.001800525056e+06	1.004551470138e+06	2.738480967159e-03
7.0e-05	1.002450980147e+06	1.007003360468e+06	4.520720088167e-03
8.0e-05	1.003201680336e+06	1.010206931359e+06	6.934471349509e-03
9.0e-05	1.004052700693e+06	1.014263203504e+06	1.006691633448e-02
1.0e-04	1.005004126320e+06	1.019273603224e+06	1.399965314356e-02

Table 1: Relative error and acceleration values for node 8 based on DYNA3D simulation and analytical derivation.

Time: t	X **Velocity**	**Analytical Value**	**Relative Error**: ϵ
0.0e+00	0.000000000000e+00	0.000000000000e+00	0.000000000000e+00
1.0e-05	5.000000000000e+00	5.000000000000e+00	0.000000000000e+00
2.0e-05	1.500050000000e+01	1.500050000000e+01	1.184198419653e-16
3.0e-05	2.500250005000e+01	2.500300005000e+01	1.999760024821e-05
4.0e-05	3.500700035001e+01	3.501000045001e+01	8.569265813879e-05
5.0e-05	4.501500135004e+01	4.502500220006e+01	2.221177018620e-04
6.0e-05	5.502750385022e+01	5.505250780039e+01	4.541836723529e-04
7.0e-05	6.504550910078e+01	6.509802250176e+01	8.066819691585e-04
8.0e-05	7.507001890225e+01	7.516805610644e+01	1.304240248629e-03
9.0e-05	8.510203570561e+01	8.527012542002e+01	1.971261489098e-03
1.0e-04	9.514256271254e+01	9.541275745506e+01	2.831851313452e-03

Table 2: Relative error and mid-step velocity values $\mathbf{v}_{n+1/2}$ for node 8 based on DYNA3D simulation and analytical derivation. The mid-step velocities were used in this comparison, because DYNA3D only outputs the mid-step nodal velocities.

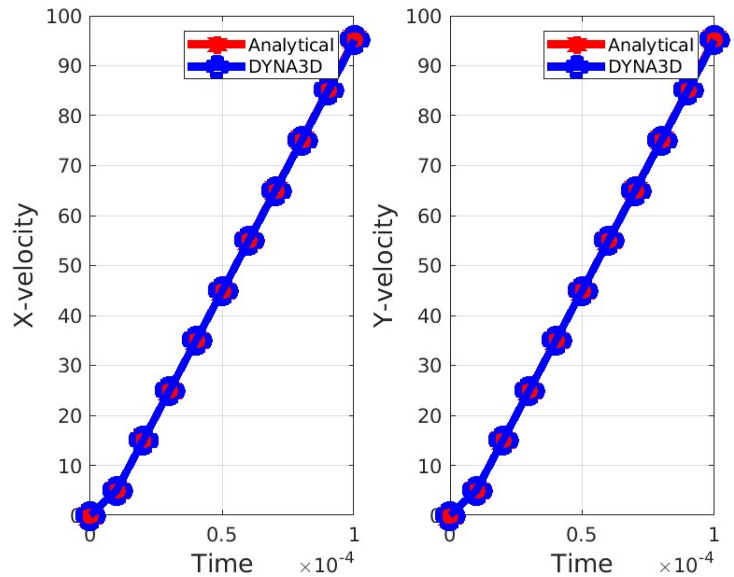


Figure 2: Comparison of the as implemented DYNA3D x and y mid-step velocity components of node 8 to the analytically derived values given the explicit time integration algorithm presented above.

Time: t	X **Displacement**	**Analytical Value**	**Relative Error**: ϵ
0.0e+00	0.000000000000e+00	0.000000000000e+00	0.000000000000e+00
1.0e-05	5.000000000000e-05	5.000000000000e-05	0.000000000000e+00
2.0e-05	2.000050000000e-04	2.000050000000e-04	0.000000000000e+00
3.0e-05	4.500300005000e-04	4.500350005000e-04	1.111024696862e-05
4.0e-05	8.001000040001e-04	8.001350050001e-04	4.374386794902e-05
5.0e-05	1.250250017501e-03	1.250385027001e-03	1.079743416907e-04
6.0e-05	1.800525056003e-03	1.800910105005e-03	2.138080078126e-04
7.0e-05	2.450980147010e-03	2.451890330022e-03	3.712168527510e-04
8.0e-05	3.201680336033e-03	3.203570891086e-03	5.901399150286e-04
9.0e-05	4.052700693089e-03	4.056272145287e-03	8.804764743690e-04
1.0e-04	5.004126320215e-03	5.010399719837e-03	1.252075677299e-03

Table 3: Relative error and displacement values for node 8 based on DYNA3D simulation and analytical derivation.

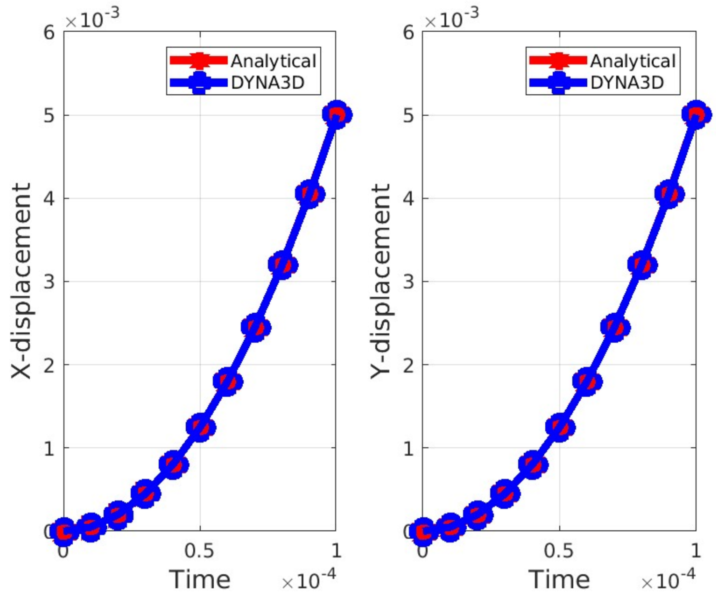


Figure 3: Comparison of the as implemented DYNA3D x and y velocity components of node 8 to the analytically derived values given the explicit time integration algorithm presented above.

3 Regression Tests

This section documents the addition of two regression tests added to the DYNA3D Software Quality Assurance test suite: `washer_rot_body_force` and `washer_eset_rot_body_force`. The two tests are almost identical to one another except for two minor differences. The first difference is that `washer_rot_body_force` applies body force loads as *global* loads, while `washer_eset_rot_body_force` applies body force loads as *element set* loads. The second difference is that `washer_rot_body_force` defines the angular velocity direction according to the specification of only 2 nodes denoting the base and tip of the direction vector, while `washer_eset_rot_body_force` defines the angular velocity direction according to the average coordinates of a collection of nodes for both the base and tip of the directional vector. The vector and chosen node labels used are shown in Figures 4 and 5. The mesh for both tests depicts a single washer consisting of 60 elements and 160 nodes, and no node enforces a Dirichlet boundary condition. Additionally, the center of rotation used in Eq. (2) is chosen to be $\mathbf{p} = (0, 0, 0)$, which coincides with the center of the washer. Each element utilizes a hypoelastic isotropic material model with material parameters: $E = 10^7$, $\nu = 0.30$, and $\rho = 10^3$. The magnitude of the angular velocity is described by the load curve,

$$\|\boldsymbol{\omega}\| = \begin{cases} t \cdot 10^5 & \text{for} \quad 0 \leq t \leq 10^{-3} \\ 10^2 & \text{for} \quad t > 10^{-3} \end{cases} . \tag{4}$$

The simulation is run for $t \in [0, 2 \times 10^{-3}]$ and variables are outputted at intervals of $\Delta t = 2 \times 10^{-4}$.

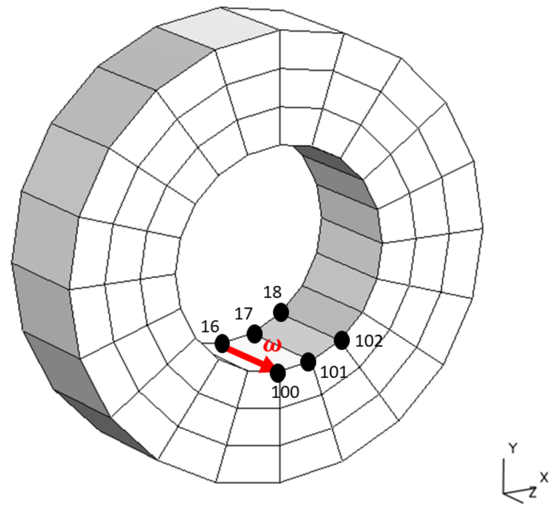


Figure 4: Mesh for regression test `washer_rot_body_force` added to SQA test suite. The angular velocity direction is defined according to nodes 16 and 100 and is illustrated above.

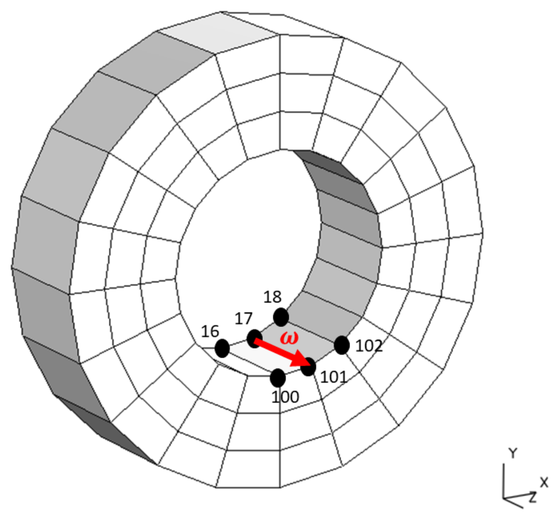
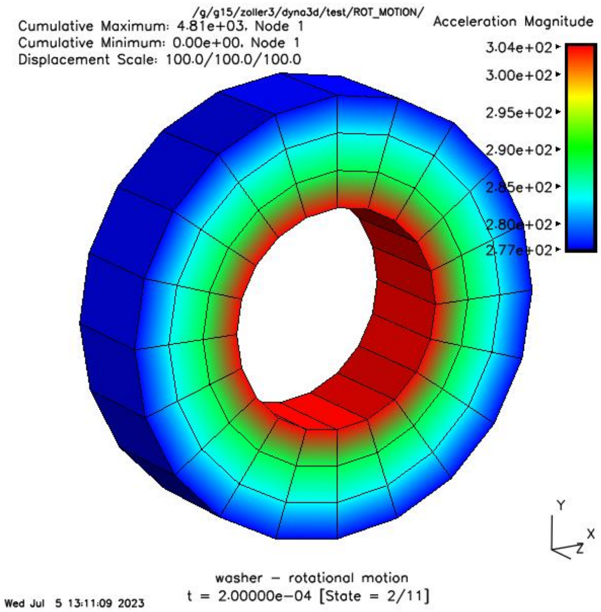
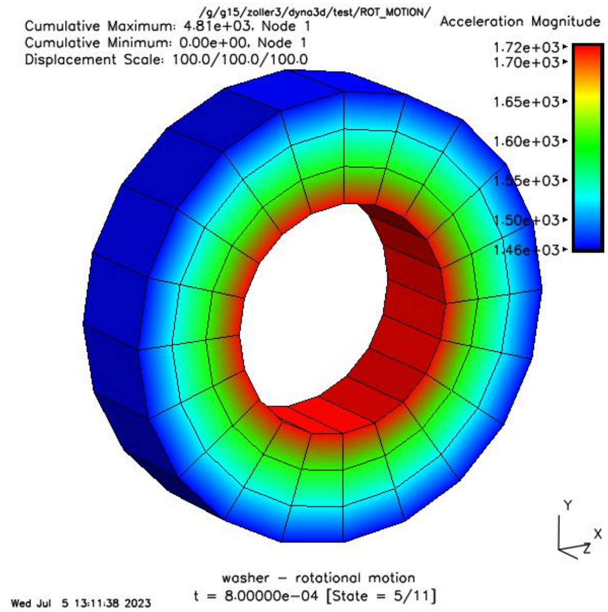


Figure 5: Mesh for regression test `washer_eset_rot_body_force` added to SQA test suite. The angular velocity direction is defined according to the set of nodes {16,17,18} and {100,101,102} denoting the average coordinates for the base and tip of $\boldsymbol{\omega}$, respectively. The resulting value of $\boldsymbol{\omega}$ is then illustrated above.

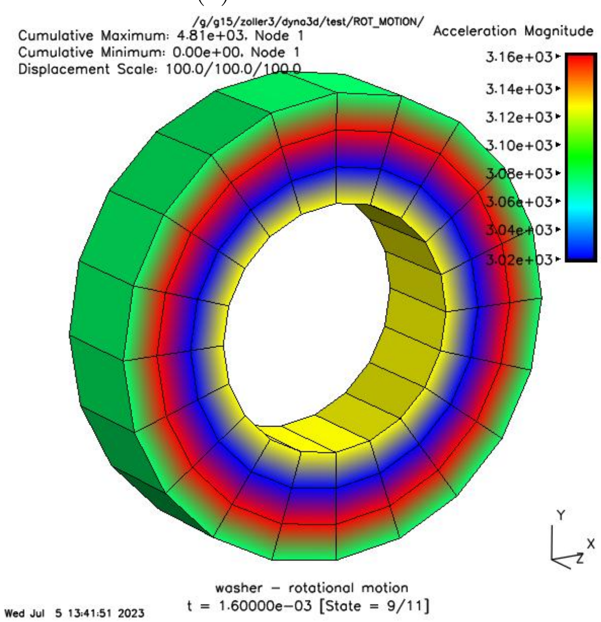
The simulation behaves as expected such that the washer expands and contracts radially due to the angular velocity $\boldsymbol{\omega}$. This phenomena is illustrated in Figures 6a-6d, where the acceleration magnitude is shown for various points in time in test `washer_rot_body_force`. The same phenomena occurs for test `washer_eset_rot_body_force` and is omitted for brevity. These two regression tests provide baseline answers for nodal displacements, velocities, and accelerations of node labels 1, 70, 101, and 164. These baseline answers help to ensure that future changes to the DYNA3D source code do not unintentionally affect the implementation of this new feature.



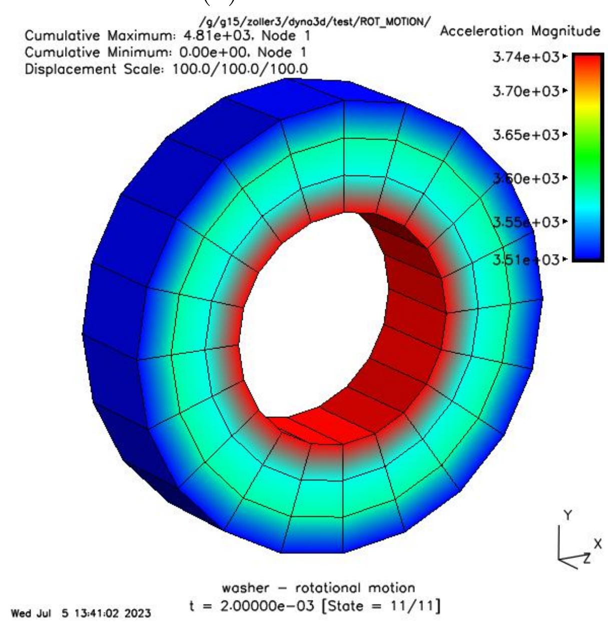
(a) $t = 2.0 \times 10^{-4}$



(b) $t = 8.0 \times 10^{-4}$



(c) $t = 1.6 \times 10^{-4}$



(d) $t = 2.0 \times 10^{-3}$

Figure 6: Acceleration magnitude at discrete points in time for regression test `washer_rot_body_force`.

4 Conclusion

In conclusion, a verification test was used and documented in this report to assess the correct implementation of a new DYNA3D feature, which applies body force loads due to a prescribed angular velocity. The test consisted of a single element and verified the feature's intended behavior. The relative errors presented in this report are unfortunately higher than expected, but this can be attributed to the neglection of the stress divergence term and proper integration over the element's spatial domain in computing analytical expressions for the nodal accelerations. These sources of error should and will be considered in future verification reports of this type. Additionally, two regression tests `washer_rot_body_force` and `washer_eset_rot_body_force` were added to the DYNA3D SQA test suite to generate baseline answers for nodal accelerations, velocities, and displacements. These tests were described above and consist of a hollow washer meshed with 60 elements and subjected to an angular velocity about its centroid. The results obtained are intuitively expected, as the washer expands and contracts given the applied body force loads.

References

T. Belytschko, W. K. Liu, B. Moran, and K. I. Elkhodary. *Nonlinear Finite Elements for Continua and Structures*. Number 2. United Kingdom, 2014. ISBN 978-1-118-63270-3.

E. Zywicz, B. Giffin, DeGroot A.J., M. Zoller, and R. Hathaway. *DYNA3D: A Nonlinear, Explicit, Three-Dimensional Finite Element Code for Solid and Structural Mechanics User Manual - Version 22*, 2022.