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Modeling Impact-Induced Reactivity Changes Using DAG-MCNP

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Abstract. There is a long literature studying the criticality of space reactors immersed in water/sand after a launch accident; however most of these studies evaluate nominal or uniformly compacted system configurations. There is less research on the reactivity consequences of impact, which can causes large structural deformation of reactor components that can result in changes in the reactivity of the system. Predicting these changes is an important component of launch safety analysis. This paper describes new features added to the DAG-MCNP5 neutronics code that allow the criticality analysis of deformed geometries. A CAD-based solid model of the reactor geometry is used to generate an initial mesh for a structural mechanics impact calculation using the PRONTO3D/PRESTO continuum mechanics codes. Boundary conditions and material specifications for the reactivity analysis are attached to the solid model that is then associated with the initial mesh representation. This geometry is then updated with the deformed finite element mesh to perturb node coordinates. DAG-MCNP5 was extended to accommodate two consequences of the large structural deformations: dead elements representing fracture, and small overlaps between adjacent volumes. The dead elements are removed during geometry initialization and adjustments are made to conserve mass. More challenging, small overlaps where adjacent mesh elements contact cause the geometric queries to become unreliable. A new point membership test was developed that is tolerant of self-intersecting volumes, and the particle tracking algorithm was adjusted to enable transport through small overlaps. These new features enable DAG-MCNP5 to perform particle transport and criticality eigenvalue calculations on both deformed mesh geometry and CAD geometry with small geometric defects. Detailed impact simulations were performed on an 85-pin space reactor model. In the most realistic model that included NaK coolant and water in the impact simulation, the eigenvalue was determined to increase 2.7% due to impact.

Keywords: Criticality, Reactivity, Space Nuclear Reactor, Deformed Geometry, CAD Import.

INTRODUCTION

Launch accidents may deform space reactors, causing a change in reactivity. Although solid models can be manually altered to approximate the shape after impact, this method is both tedious and limited in accuracy. An alternative approach has been developed which utilizes mesh geometry exported by a structural dynamics simulation. Mesh-based radiation transport enables high-fidelity geometric description of deformed CAD models. This work resulted in a time-dependent reactivity assessment of a space reactor impacting a concrete pad after launch failure.

The Monte Carlo N-Particle (MCNP) radiation transport code was selected to determine the reactivity of the system [Girard]. The Direct Accelerated Geometry for Monte Carlo (DAGMC) library, developed at the University of Wisconsin, evaluates geometric queries for MCNP directly on the CAD geometry [Tautges et al.]. Referred to as DAG-MCNP5 when coupled with MCNP5, it has been used for many

fusion and fission applications featuring complex CAD geometry [Sawan et al.]. In this work, deformed finite element mesh models are initialized to create DAGMC-compatible geometry. New capability was added to DAGMC including *mesh-based geometry initialization* and *overlap-tolerant particle tracking*.

Structural failure presents a unique challenge when initializing deformed mesh geometry for DAGMC. During impact, mesh elements may experience structural forces that result in fracture. Mesh elements lose their stiffness to simulate fracture causing them to become geometrically invalid. Labeled as *dead*, these elements cease to participate in the remainder of the structural analysis. Adjusting the mesh topology to remove dead elements requires special treatment.

The particle tracking algorithm required adjustment due to contact of adjacent bodies in the structural analysis. When calculating contact, the structural analysis permits small overlap of adjacent bodies. When initialized for DAGMC, small overlaps result in self-intersecting volumes. Common point membership tests fail for self-intersecting volumes. Small overlaps are problematic for particle tracking because the next surface intersection may exist slightly behind the particle's geometric position. Although overlaps are small enough not to affect the physics of the simulation, additional logic is required for successful particle tracking.

An 85-pin space reactor concept was used to demonstrate the capabilities developed, as shown in Figure 1 [Marcille et al.]. UO_2 fuel pins are clad in SS316 and cooled by NaK. Six control drums containing B_4C and Be are positioned around the perimeter of the core inside a 15.3 cm radial Be reflector. The 25 kW_e reactor is shielded by borated water. The fueled core is 38 cm high with a diameter of 22.9 cm. The structural components of the reactor are SS316. Additional engineering details were added as described by Villa et al.

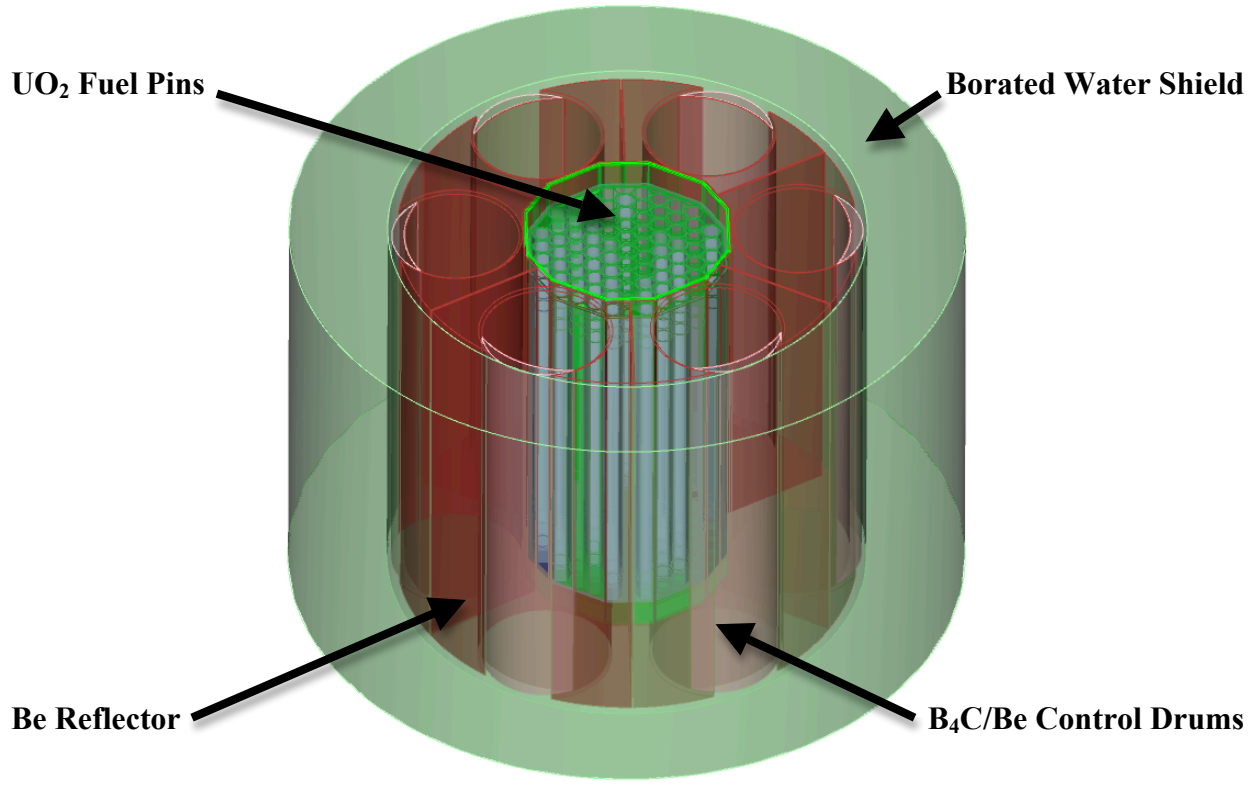

FIGURE 1. Space Reactor Proposed by Marcille et al.

GEOMETRY INITIALIZATION

Model creation and structural analysis were performed by Villa et al. A solid model of the reactor geometry was created in the Cubit geometry and mesh generation toolkit [Clark]. Structural components were meshed with hexahedral elements. The mesh was exported from Cubit using the Exodus II file format [Schoof and Yarberry]. Optionally, fluid volumes were filled with smoothed particle hydrodynamics (SPH) elements using tools developed by Villa et al. The PRONTO3D/PRESTO continuum mechanics codes were used for structural analysis. The output of the structural analysis was an Exodus II file of the deformed mesh.

After structural analysis the model was prepared for reactivity analysis. Additional geometry was specified to define reflective and absorbing boundary conditions around the deformed model. Boundary conditions and materials were specified by assigning groups to the solid model within Cubit. An MCNP5 input file was created with material definitions and other data cards, but no cell or surface cards. The MCNP5 input file, Cubit geometry file, and Exodus II deformed mesh file were needed to perform a reactivity analysis. Geometry initialization includes the following steps:

- reading the undeformed solid and mesh models from the Cubit file,
- updating the mesh node locations from the deformed mesh model in the Exodus II file,
- removing dead elements from the mesh,
- converting quadrilaterals to triangles, and
- adjusting material densities to accommodate volume changes.

A geometry initialization routine was used to convert the output of the structural analysis into a DAGMC-compatible file. First the Cubit file was read to extract the solid and mesh models. The surfaces of the solid model were associated with the corresponding surfaces of the mesh model, using global IDs. A uniform surface sense was established for each pair of corresponding solid/mesh surfaces. This ensured that corresponding surfaces of the solid and mesh models have the same orientation.

Next the deformed model was read. Associations between nodes in the mesh model and deformed model were created using global IDs. Node coordinates of the mesh model were updated with positions from the deformed model.

Dead mesh elements were removed from the mesh model. Using topology, the bounding faces of the mesh model were identified. Some of the bounding faces were altered by removal of dead mesh elements. New surfaces were created for mesh faces that did not belong to original surfaces of the mesh model.

If corresponding surfaces existed, surfaces of the solid model were replaced by surfaces of the mesh model. This preserves surfaces of the solid model belonging to boundary conditions that did not exist in the mesh model, including reflecting and absorbing boundaries. Quadrilateral elements were converted to triangles by splitting along the shortest diagonal. Surfaces were removed if they no longer contained any mesh faces. Volumes were removed if all of their surfaces have been removed.

Volumes of structural components changed due to element death and material compressibility. The density of each volume was adjusted so that mass was conserved during the deformation. The solid model faceted with a tolerance of 1 μm was used to determine the undeformed volume. The facet tolerance is the maximum distance between the faceted surface and the continuous surface of the solid model. Geometry initialization steps for DAGMC are described with more detail in Smith et al.

To illustrate the geometry initialization, Figure 2 shows a structural steel component of the 85-pin model pre/post deformation. Figure 2 (left) displays the Cubit hexahedral mesh as input to the structural analysis. Figure 2 (right) shows the deformed geometry as initialized for DAGMC. The node coordinates have been updated to their deformed locations. Dead elements have been removed, leaving a void. A new

surface (yellow) has been created with mesh faces exposed by removing dead elements. Quadrilateral mesh faces have been converted to triangles.

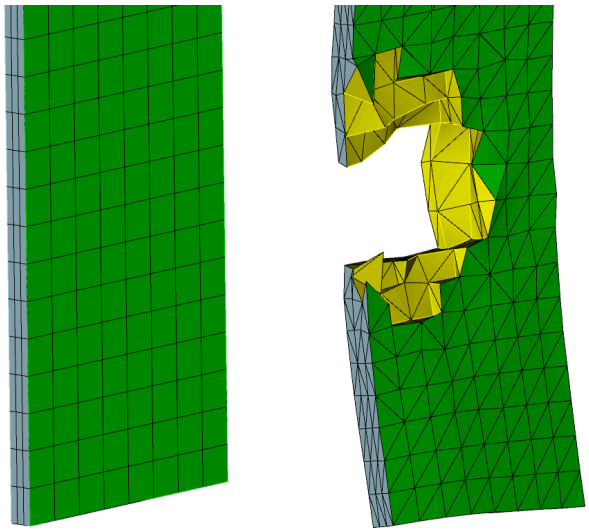

FIGURE 2. 0-Degree SPH Model's Undeformed Cubit Mesh (left) and DAGMC-Initialized Geometry at 0.225 ms (right).

PARTICLE TRACKING

The geometric model created by the initialization routine is in the form of a boundary representation. The solid model consists of geometric volumes, surfaces, curves, and vertices. Geometric entities are represented by meshed entities, including elements, faces, edges, and nodes. DAGMC only utilizes volumes and surfaces. Volumes are represented by their bounding surfaces. Surfaces are represented as sets of mesh faces. Mesh faces are triangles specified by three nodes. Mesh faces of each surface have uniform orientation, and geometric surfaces have consistent orientation with respect to parent volumes. The undeformed boundary of each volume is a manifold. However, surfaces may be shared by two volumes, creating a non-manifold model.

After deformation the boundary of a volume may contain self-intersections due to imprecise contact calculation of the structural simulation. These defects violate assumptions in the algorithms for determining whether a volume contains a point and finding ray-surface intersections; new algorithms were developed for both of these. Self-intersections can also be caused by imperfect draftsmanship and file translation of CAD models. Before this work, these errors were tedious to repair, requiring extensive manual labor. The ability to perform particle transport through geometry with small defects will enable deformed mesh analysis and streamline traditional CAD model analysis.

A point membership test is used to determine the volume that source particles start inside. Because the existing test in DAGMC is not tolerant of self-intersecting volumes, a new point membership test was developed. To conduct the test, a ray is cast from the point in any direction. The traditional ray crossing method uses the number of surface intersections to determine point membership. The proposed *ray crossing with orientation* method uses the orientation of each surface crossing to sum the exit/entrance nature of intersections along the ray. A point that is inside the volume will have at least one more exit than entrance. It is unlikely but possible that the ray intersects an edge or node between triangles. This situation is resolved by examining the triangles in the neighborhood of the edge or node intersection.

An overlap-tolerant particle tracking algorithm was developed to find surface intersections, even if the next surface is behind the particle's current position. The tracking algorithm searches for the intersection

at which a particle leaves the current volume, known as the *exit intersection*. After geometry initialization, each surface is adjacent to exactly two volumes. When a particle leaves the current volume, the next volume is determined using surface adjacency information. The tracking algorithm then searches for the exit intersection of the next volume. Only exit intersections are found because the ray's exit intersection of the current volume is identical to the entrance intersection of the next volume.

Self-intersecting volumes present a challenge because the exit intersection may occur behind the particle's geometric position. This allows the geometric position (its coordinates in space) and logical position (the volume it is in) of a particle to become inconsistent. If an overlap is detected, the logical position must be updated without a corresponding change in geometric position. This is valid because the overlap thickness is assumed to be small enough to not significantly affect the physics of the simulation. Several other techniques are used to ensure accurate tracking including triangle orientation checks, storing previously intersected triangles along a streaming path, and occasionally performing point membership tests to check for overlap.

REACTIVITY CALCULATIONS

A comparison was performed between native MCNP5 and the overlap-tolerant version of DAG-MCNP5 using an undeformed solid model. The 85-pin space reactor was analyzed with control drums rotated for minimum neutron absorption. MCNP native geometry was converted to ACIS-formatted CAD geometry using the MCNP2CAD automated conversion utility. Material properties and boundary conditions were automatically mapped to the CAD file. The model has 1176 volumes and 4947 surfaces. Merging of coincident surfaces in the solid model was not required due to the overlap-tolerant tracking algorithm. Surfaces of the solid model were faceted with a tolerance of 1 μm. Both cases had 10 inactive cycles, 100 active cycles, and 10,000 source neutrons per cycle. The native MCNP5 case had a k_{eff} of 1.01437 (±0.00075). This compares well with the DAG-MCNP5 k_{eff} of 1.01451 (±0.00080).

Three simulations were performed of the 85-pin reactor impacting concrete at 100 m/s by Villa et al., as shown in Table 1. Simulations were performed at two different angles of impact, measured between the reactor's vertical axis and the surface normal vector of the concrete pad. At 0-degrees, one case included the effects of fluids in the structural analysis using SPH elements, but neither included fluids in the reactivity analysis. At 45-degrees, the fluids were excluded from both the structural and reactivity analyses. Although DAGMC cannot utilize SPH elements, adding fluids increases the accuracy of the impact simulation. For efficiency, 1/2 and 1/12 symmetry were used for the 0-degree and 45-degree models respectively. The volume, surface, and triangle count in Table 1 are from the last time step of the deformation, once initialized in DAGMC. The hexahedra count references the Cubit mesh because hexahedra do not exist in the DAGMC-initialized geometry. The particle tracking rate is representative of one core on a 2.66 GHz Intel Core2 processor and has been averaged for all cases. The computational time required for structural analysis was decreased by doubling the thickness of the cladding to 0.1 cm. Control drums were rotated for maximum neutron absorption. Material density was adjusted to conserve mass on a per-volume basis, despite element volume change and the removal of dead elements.

Selected time steps for each model were analyzed as a series of DAG-MCNP5 cases. Each case had 10 inactive cycles, 100 active cycles, and 10,000 source neutrons per cycle. Depending on the particle tracking rate, each case took 5-7 hours on one core of a 2.66 GHz Intel Core2 processor. During geometry initialization, some poorly formed quadrilateral faces were converted into intersecting triangles. Intersecting triangles create a non-orientable surface, causing lost particles. The average lost particle fraction was 3.3×10^{-6}. The neutron multiplication factor is shown for each simulation in Figure 3. Error bars represent one standard deviation, but are small compared to the impact-induced change in k_{eff}.

TABLE 1. Summary of 85-Pin Reactor Impact Models.

Angle	SPH	Symmetry	Entity Count				Tracking Rate
[degrees]			Vols.	Surfs.	Hex.	Tris.	[particles/min]
0	No	1/12	1308	6673	962k	1.43M	3793
0	Yes	1/12	3181	17867	966k	1.51M	3137
45	No	1/2	3176	11729	8.86M	11.1M	2741

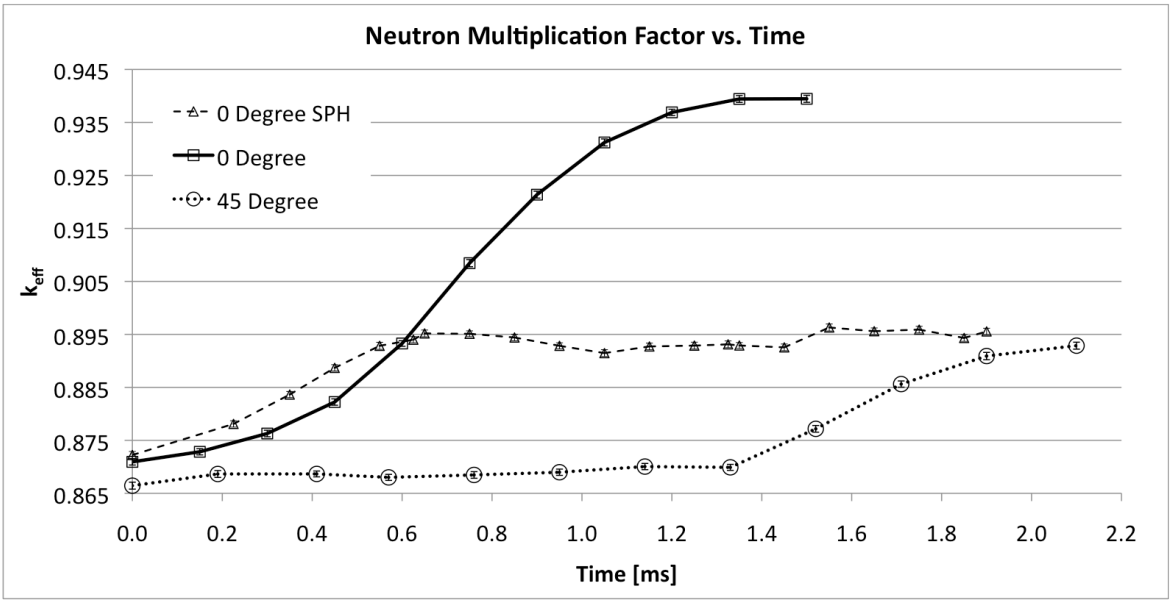

FIGURE 3. Time-Dependent Neutron Multiplication Factor.

The 0-degree simulation without SPH elements had the greatest increase in k_{eff}. NaK coolant and water shielding were added to the 0-degree structural simulation through the use of SPH elements. The reactivity simulations did not include fluids. Figure 4 contrasts the 0-degree simulations with and without SPH elements. Green SPH elements model water shielding and orange SPH elements model NaK coolant. Water SPH elements cause the shield containment to break. The inclusion of fluids in the structural simulation restricts the increase of k_{eff} by limiting contact of adjacent fuel pins toward the bottom of the reactor. The NaK dampens impact by absorbing kinetic energy that would otherwise deform fuel and structural components. The structural analysis is explained in more detail by Villa et al. and Smith et al. Despite the additional challenge of including fluids in the structural simulation, this work suggests they are crucial to producing realistic results.

Although computational expense did not permit the inclusion of SPH elements, a 45-degree collision was simulated, as shown in Figures 3 and 5. Although the simulation did not extend until all kinetic energy was dissipated due to time constraints, it clearly demonstrates predictive capability. The neutron multiplication factor did not increase for the first 0.95 milliseconds of impact because the fuel pins did not move relative to one another. Compared with the 0-degree simulation, the increase in k_{eff} occurred later in the 45-degree simulation due to the angle of impact. After 0.95 milliseconds the distance between fuel pins began to decrease with a corresponding increase in k_{eff}, as shown in Figure 3.

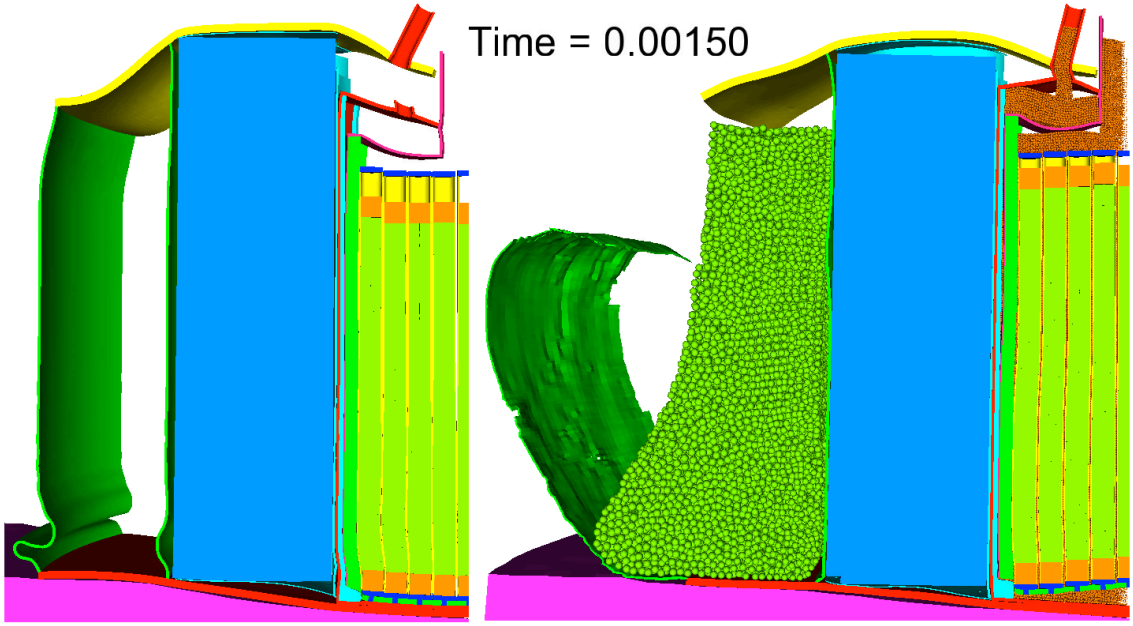

FIGURE 4. 0-Degree Impact at 1.5 ms without (left) and with (right) SPH Elements. Image from Villa et.al.

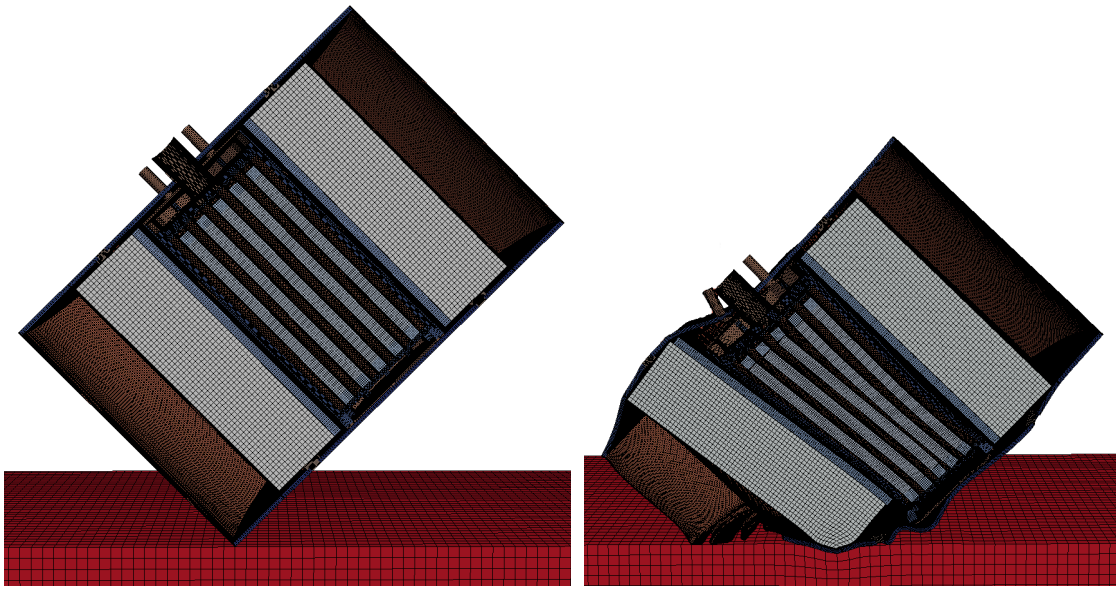

FIGURE 5. 45-Degree Impact at 0.0 ms (left) and 2.1 ms (right).

The effect of neglecting fluids in the reactivity simulations has been estimated. The surfaces that bound fluid volumes puncture due to fracture in the structural simulation. Fluids cannot be modeled as a continuous material without being contained in a closed volume. An alternative approach would model fluids as spherical volumes, analogous to SPH elements in the structural simulation. To determine the effect of neglecting fluids in the reactivity analysis, water shielding and NaK coolant were added to the undeformed solid model with control drums rotated for maximum neutron absorption. The neutron multiplication factor increased from 0.87112 (±0.00069) to 0.87987 (±0.00064) when fluids were included. This suggests that for the 85-pin model, neglecting fluids in the reactivity analysis decreases k_{eff} by about 1%.

CONCLUSION

An initialization routine was added to DAGMC that enabled radiation transport on deformed mesh geometry. A new point membership test and tracking algorithm were developed to tolerate small overlaps caused by contact of neighboring mesh elements. These tools were used to explore time-dependent reactivity during impact. Structural simulations were performed of the reactor impacting concrete at 100 m/s with impact angles of 0 and 45 degrees. NaK coolant and borated water shielding were included in a 0-degree structural simulation to examine the effect of fluids during impact. Deformed geometry was initialized for reactivity assessment without including fluids. The neutron multiplication factor increased 2.7% and 7.7% for the 0-degree impact with and without fluids in the structural simulation, respectively. The neutron multiplication factor increased 3.0% for the 45-degree simulation, which did not include fluids. In all cases the reactor remained subcritical due to the substantial amount of subcriticality at launch. The accuracy of these results depends on assumptions made in the structural and reactivity simulations. Material properties, dead element handling, and fluid inclusion in the reactivity simulation are opportunities for improvement.

ACKNOWLEDGMENTS

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