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Modeling Impact-Induced Reactivity Changes Using DAG-MCNP

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Outline

Although Rare, Launch Failures Do Occur

- After successful launch, space reactors provide high-density, continuous power
- Not all launches are successful
- Reactor may deform due to impact
- Predicting reactivity change due to impact is an important component of launch safety analysis

http://www.g2mil.com/safety.htm

Reactivity Analysis of Deformed Geometry is Difficult

Previous Efforts

- Approximate deformed shape by manually altering geometry
- Examine water/sand immersion at nominal or uniformly compacted density
- Significant manual effort with limited accuracy

Our Approach

- Structural analysis uses a finite element model (FEM) for high-fidelity geometric description
- DAGMC is optimized for facet-based models (FBMs)
- DAG-MCNP can be used to predict reactivity consequence of impact

Direct Accelerated Geometry: DAG-MCNP

DAG-MCNP is a coupling of the Mesh Oriented datABase (MOAB) and Monte Carlo N-Particle (MCNP) software packages [Tautges et al., 2009]

Software

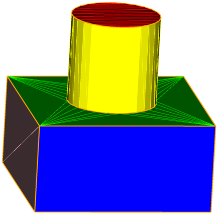
- Common Geometry Module, Argonne (CGMA): geometry library, C++, open source
- MOAB: mesh library, C++, open source
- MCNP: physics code, FORTRAN, from LANL

Implementation

1. CGMA loads models with ACIS or OCC
2. MOAB calls CGMA to facet model
3. MCNP calls MOAB to perform geometric queries

Geometry Model: **Faceted CAD Data**

- Volumes, surfaces, curves, vertices
- Non-manifold surfaces
- Solid model→faceted model



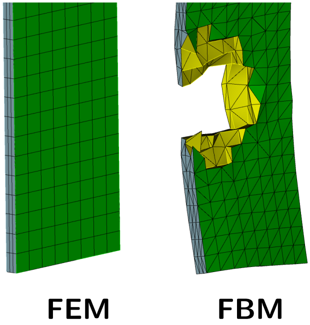
Deformed Geometry Challenges

- Convert FEM→FBM
- Dead Elements (fracture)
- Element Volume Change
- Overlapping Volumes

New Feature: Mesh Geometry Initialization

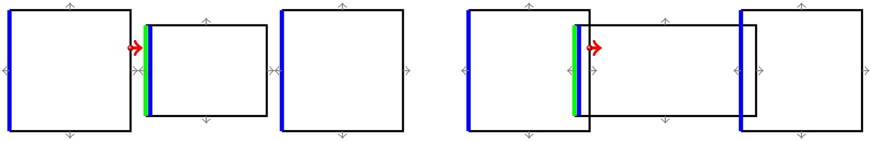
Procedure

1. Load CAD model and facet surfaces
2. Load mesh model and, if they exist, replace faceted surfaces with mesh surfaces
3. Update node locations with coordinates from deformed mesh model
4. Remove *dead elements* from the mesh and recover affected surfaces
5. Converted quadrilateral mesh faces to triangles
6. Adjust material densities to accommodate volume changes



Contribution: Automatically convert deformed hexahedral mesh to facet-based model for DAGMC

Overlap Tolerance



No Overlap **Overlaps**

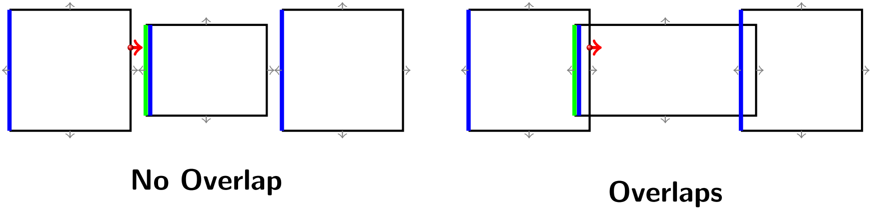
- Overlaps due to imprecise contact calculation in structural simulation, file translation, imperfect draftsmanship

  Assumption Overlaps are small enough to not significantly affect physics

- Monte Carlo packages lose all particles that encounter overlaps

  Solution improve draftsmanship, avoid translation, repair manually, change tracking algorithm

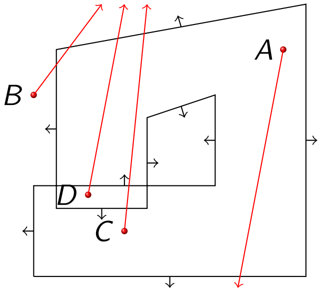
New Feature: Overlap-Tolerant Particle Tracking



- For efficiency, DAGMC only searches the current volume for exit intersections
- Search behind the ray origin for exit intersections
- Correct orientation is necessary, but not sufficient
- If overlap, particle will be inside next volume

Result: Move particle zero distance to bring logical position (the volume it is in) and geometric position (its coordinates in space) into agreement.

New Feature: Overlap-Tolerant Point Inclusion Test



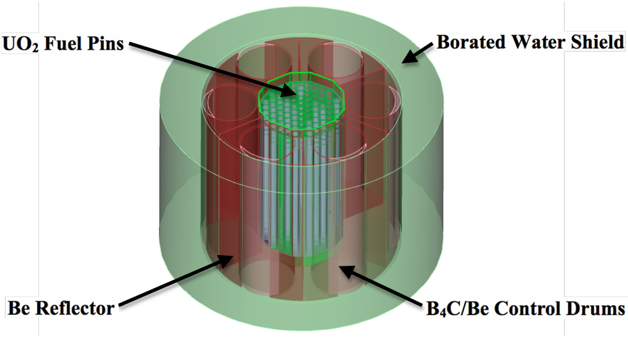
Test Point	Old Method	New Method
A	*inside*	*inside*
B	*outside*	*outside*
C	~~*outside*~~	*inside*
D	*inside*	*inside*

- Point inclusion test used to start source particles & tracking
- *Ray intersection method* compares direction of ray with surface normal at closest intersection

  Problem: The exit/entrance of first intersection is unreliable, due to self intersections
- Instead, sum all entrance/exit intersections along ray to ∞
- *Inside* points will have at least one more exit than entrance

85-Pin Space Reactor [Marcille et al., 2006]

- 25 kW_e core is 38 cm high, 22.9 cm diameter
- UO_2 fuel pins clad in 316 SS and cooled by NaK
- Six B_4C/Be control drums inside 15.3 cm radial Be reflector
- Surrounded by borated water shield
- Structural components are 316 SS
- Engineering details added as described by [Villa, 2011]

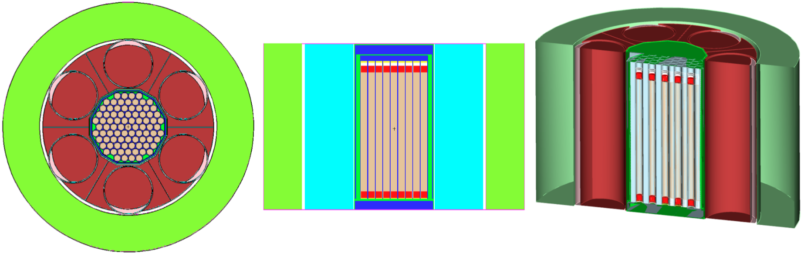


Analysis Workflow

1. Create CAD model and mesh in CUBIT
2. Optional: fill fluid volumes with SPH elements
3. Perform structural analysis with PRONTO3D/PRESTO
4. Perform reactivity analysis with DAG-MCNP
   - Assign boundary conditions and materials to CAD model within CUBIT
   - Create MCNP input file containing only data cards—no cell or surface cards
   - Initialize deformed mesh model for DAGMC
   - Determine k_{eff} using DAG-MCNP

Model creation and structural analysis performed at SNL by Villa et. al.

Compare Native MCNP vs. DAG-MCNP



- 85-pin space reactor with control drums rotated for minimum absorption
- Automated conversion of geometry, materials, and boundary conditions from MCNP geometry to ACIS CAD geometry
- Intentionally forced CAD model to have coincident, overlapping surfaces
- Used to validate Overlap-tolerant logic before analyzing deformed geometry

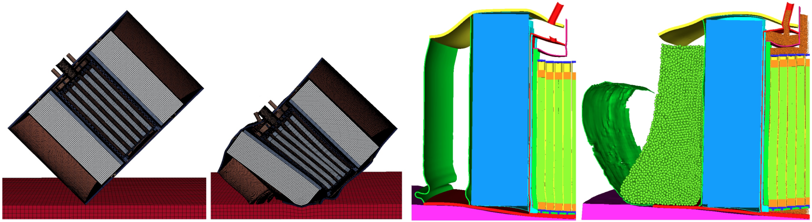
Native MCNP5

- Native geometry
- $k_{eff} = 1.01437$ (± 0.00075)

DAG-MCNP5

- CAD Geometry, $\varepsilon_f = 1\ \mu$m
- $k_{eff} = 1.01451$ (± 0.00080)

Deformed Reactor Simulations



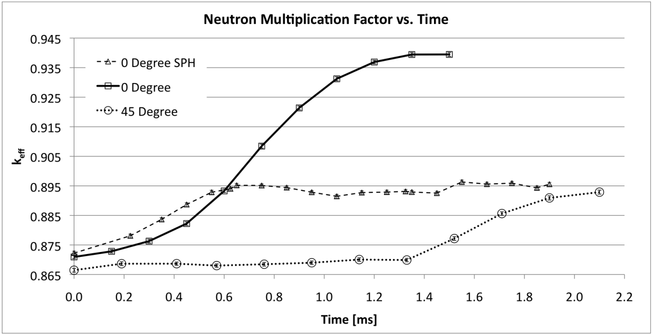
45-degree 0 ms — 45-degree 2.1 ms — 0-degree 1.5 ms — 0-degree SPH 1.5 ms

Simulation	Angle [degrees]	SPH	Symmetry	Entity Count Vol.s	Surfs.	Hex.	Tris.	Tracking Rate [part./min.]
1	45	no	1/2	3176	11729	8.86M	11.1M	2741
2	0	no	1/12	1308	6673	962k	1.43M	3793
3	0	yes	1/12	3181	17867	966k	1.51M	3137

- Reactor impacts concrete impact at 100 m/s
- Fluids modeled in 0-degree structural analysis using SPH particles
- Fluids not modeled in reactivity analysis
- Control drums rotated for maximum absorption
- First known mesh-based effort to model deformed reactors

Reactivity

- Each DAG-MCNP5 case required 5-7 hours on one core of 2.66 GHz Intel Core2
- Error bars (small) indicate 1 standard deviation



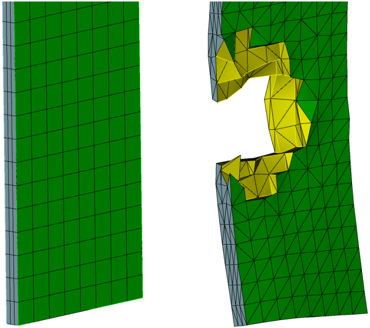
Discussion

- 45-degree simulation: k_{eff} did not increase until ∼1 ms when fuel pins moved relative to one another
- 0-degree SPH simulation: SPH elements limit contact of adjacent fuel pins→restrict increase in k_{eff} to 2.7%

Effect of Fluids in Reactivity Analysis

- Boundaries of fluid volumes puncture due to fracture→fluids mix
- Water shielding and NaK coolant not modeled in reactivity analysis
  - Future work: use SPH elements in reactivity analysis
- Use undeformed CAD model to estimate effect of fluids
  - Fluids: k_{eff}=0.87987 (0.00064)
  - No Fluids: k_{eff}=0.87112 (0.00069)
- For reactivity calculation, fluids increase k_{eff} by ∼0.01

Lost Particles Caused by Non-Orientable Surface



- Intersecting faces created when converting quadrilaterals to triangles
- Resulting surface is non-orientable
- Volume boundary is ill-defined, causing lost particles
- Average lost particle fraction is $3.3\text{x}10^{-6}$

Summary

- DAG-MCNP used to determine k_{eff} of complex deformed mesh geometries
- Fluids in the structural simulation are crucial for producing realistic results
- More work is needed to understand the effect of fluids in the reactivity analysis
- In the most realistic simulation, k_{eff} increases 2.7%
- Reactor remains subcritical, due to substantial subcriticality at launch

Extensions

- Simplify workflow to depend only on deformed mesh file
- Simulate fluids in reactivity analysis, possibly with SPH elements
- Improve conversion of deformed quadrilateral faces to triangles

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Questions?

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