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Title: Critical Experiment Benchmark Results using UM and Mesh Quality Recommendations

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Web

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Critical Experiment Benchmark Results using UM and Mesh Quality Recommendations

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Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

Critical Benchmarks using UM Geometry

- Model Criticality Benchmarks using MCNP6.2 UM
  - **HEU-MET-FAST-001**: Godiva, a bare, fast, spherical assembly of highly enriched uranium metal, 94% ^{235}U.
  - **HEU-MET-FAST-007-037**: Highly enriched uranium metal slabs moderated with polyethylene and reflected with polyethylene.
  - **IEU-MET-FAST-007**: Big Ten, a large, mixed-uranium cylindrical core with 10% average ^{235}U enrichment, surrounded by a thick ^{238}U reflector.
  - **PU-MET-FAST-022**: A bare, fast, spherical assembly of delta-phase plutonium metal, 98% ^{239}Pu.
  - **PU-SOL-THERM-001-001**: A water-reflected 11.5-inch diameter sphere of plutonium nitrate solution.

It is possible to generate a mesh, which for most purposes reflects the geometry adequately, and yet does not properly preserve mass and/or volume to the degree necessary for correct criticality calculation leading to incorrect k-effective results

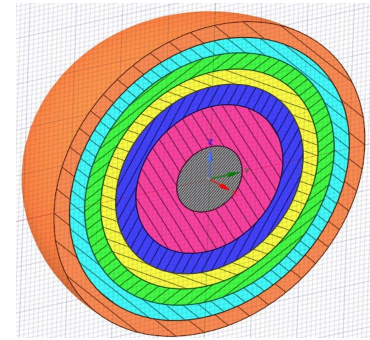
Determine engineering best practices for mesh parameters

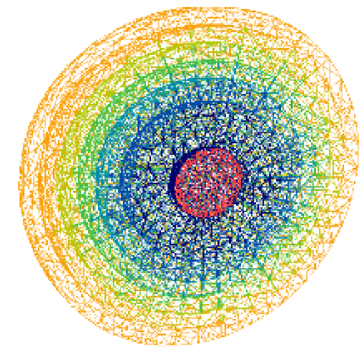
- Mesh within mass and/or volume tolerances → 1-2%
  - Volume within 2%, SA/V within 1%, density adjustment refinement
- Provide description of expert techniques
- Compare MCNP6.2 CSG, UM results and experiment results → bias within 1% of experiment

Critical Benchmarks- UM Geometry

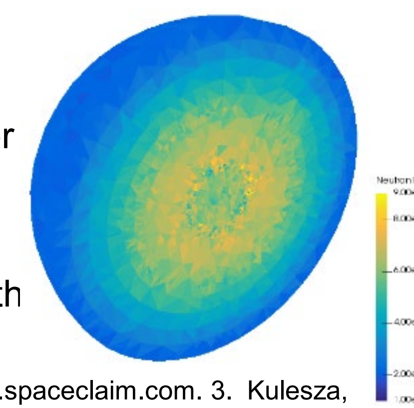
Study used of Attila4MC[1] with:

1. Construct a solid geometry using SpaceClaim[2],
2. Import a solid geometry into the Attila4MC project,
3. Create a mesh using Attila4MC,
4. Specify a calculation using the Attila4MC graphical user interface, create MCNP6.2 input file and Abaqus mesh file
5. Modify MCNP6.2 input file to specify kcode parameters,
6. Execute MCNP6.2 kcode calculation, pass statistical & convergence checks,
7. Compare calculated k-effective result with experiment result, and
8. Convert .eeout to .vtk[3] & visualize with Paraview[4].





Note: May use Abaqus[5]. This study uses Attila4MC to generate Abaqus file, the engineering best practices offered should apply equally well, regardless of whether the model construction method uses Attila4MC or Abaqus to generate the Abaqus mesh file.

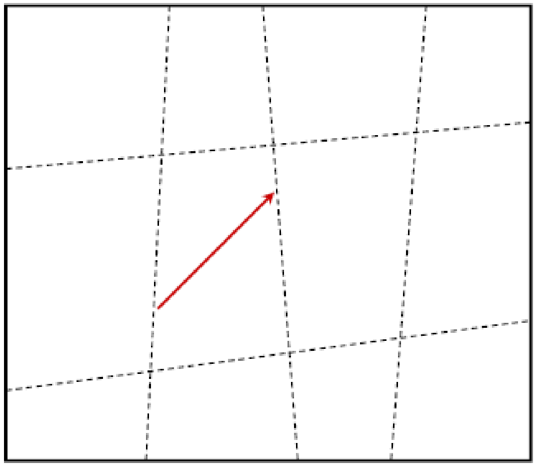


*Study uses 1st order tetrahedral elements, 2nd order elements may be efficient with regard to curvature, the same engineering best practices apply

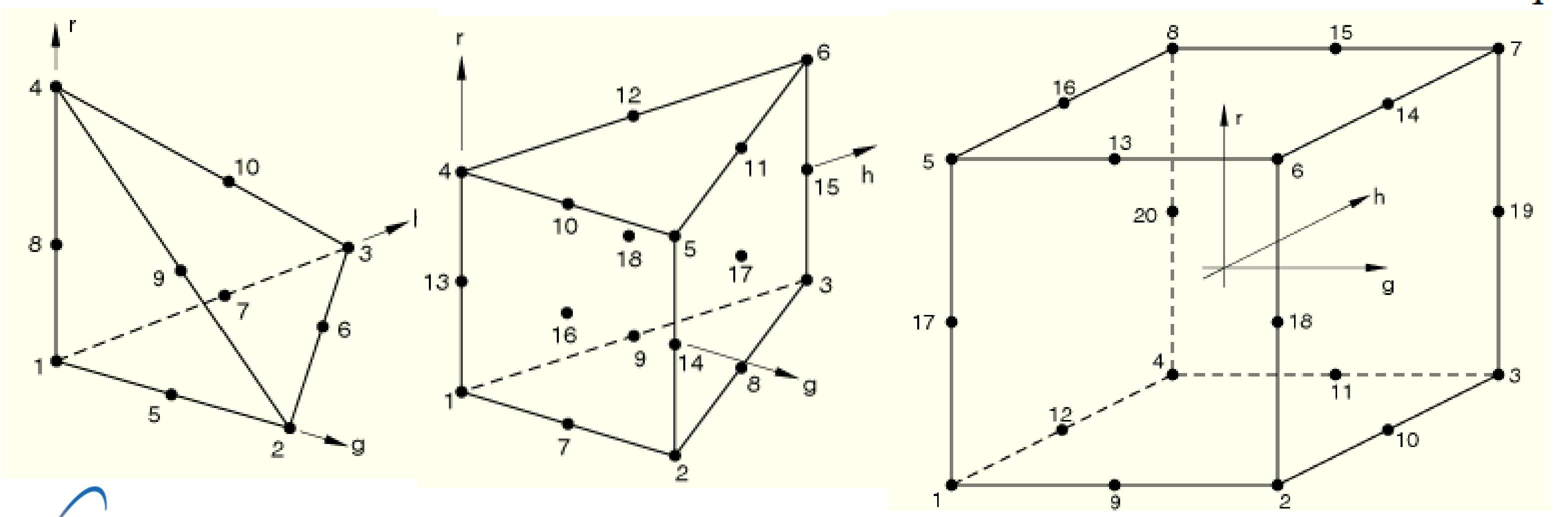
1. Attila4MC. Attila User's Manual, Varex Imaging. 2. SpaceClaim. ANSYS SpaceClaim, www.spaceclaim.com. 3. Kulesza, Joel. A Python Script to Convert MCNP Unstructured Mesh Elemental Edit Output Files to XML-based VTK Files. Los Alamos National Laboratory, LA-UR-19-20291. 2019. 4. The Paraview Guide, Kitware, Inc, www.Paraview.org, /Paraview-guide. 5. Abaqus. Dassault Systems. Abaqus Unified FEA. www.3ds.com/products-services/similia/products/abaqus

UM Geometry

- Nodes- vertices (1st order); vertices and edges (2nd order)
- Faces- sides
- Edges
- Elements
- Unstructured polyhedrons with 4-,5-, and 6- sides. Surfaces may be bilinear or quadratic depending on the number nodes

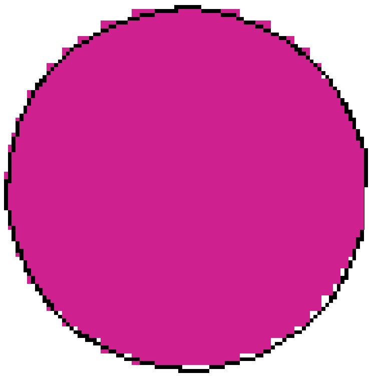


12-element part

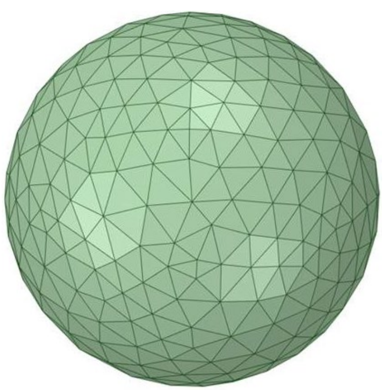


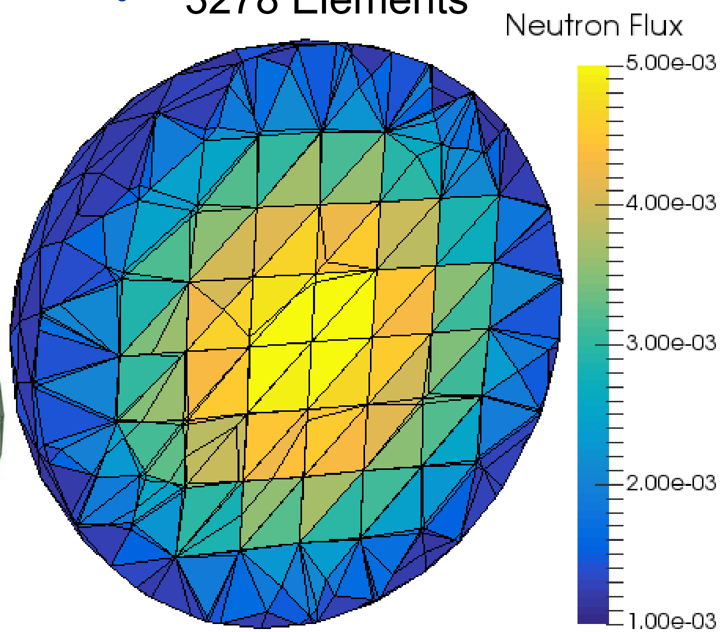
HMF001: Godiva

Benchmark	CSG % Diff	UM % Diff	C/E CSG	C/E UM
HEU-MET-FAST-001	0.00%	-0.16%	1.0000	0.9984



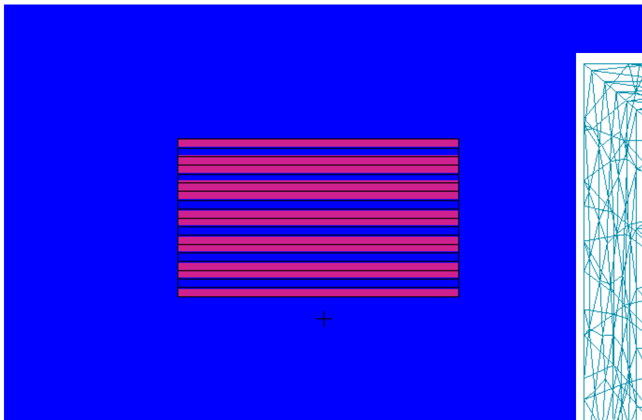
- 762 Nodes
- 668 Faces
- 3278 Elements

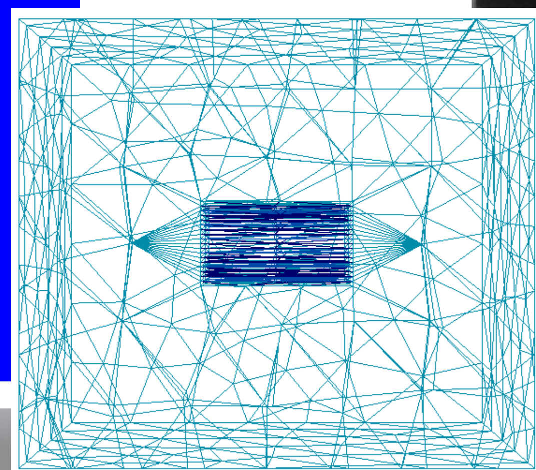


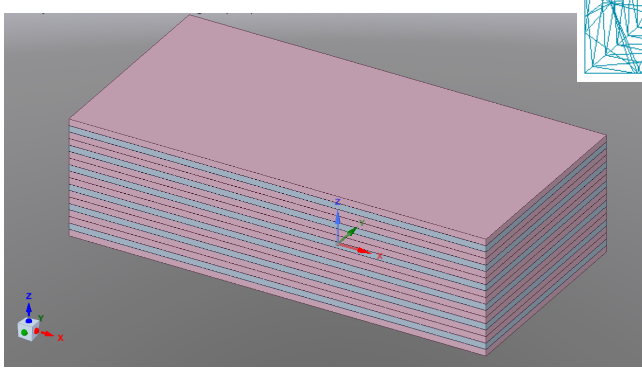


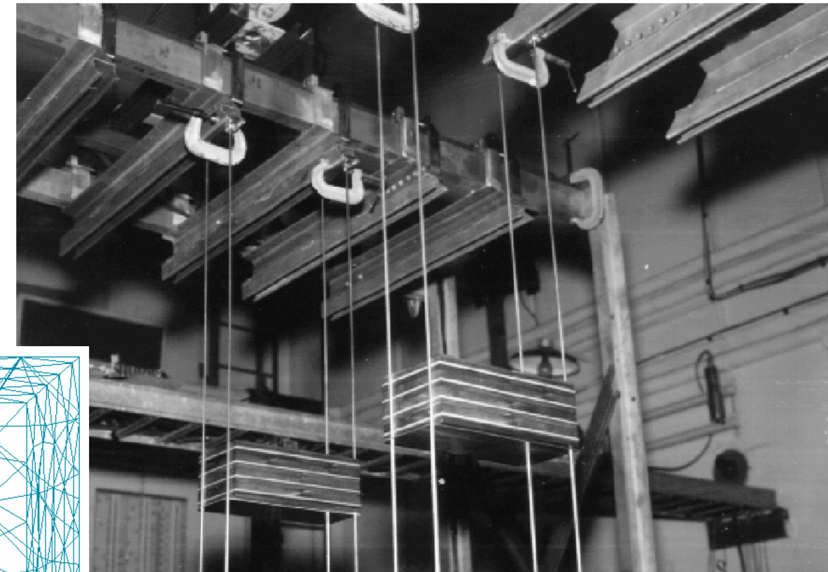
HMF007-037

Benchmark	CSG % Diff	UM % Diff	C/E CSG	C/E UM
HMF-007-037	0.30%	0.29%	1.0030	1.0029





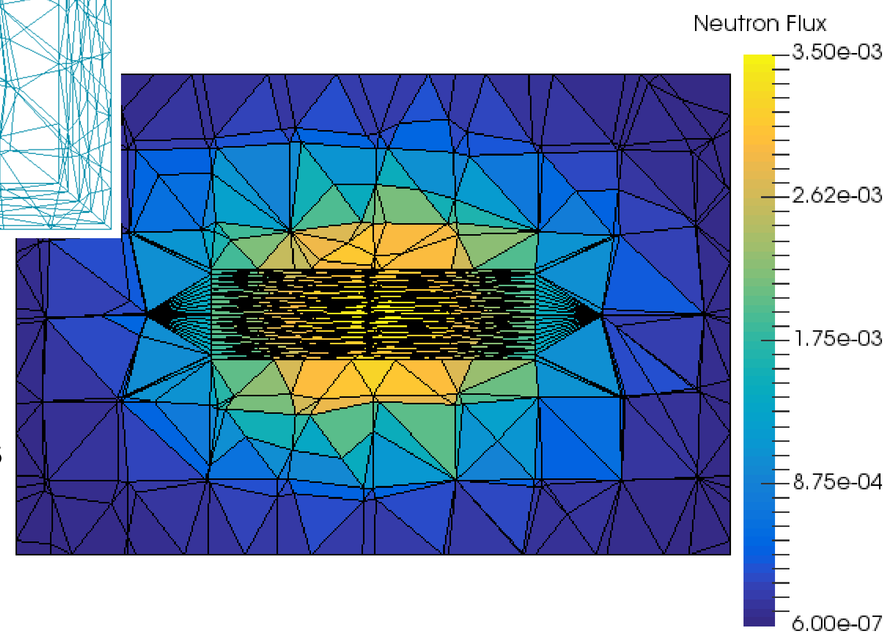




1419 Nodes

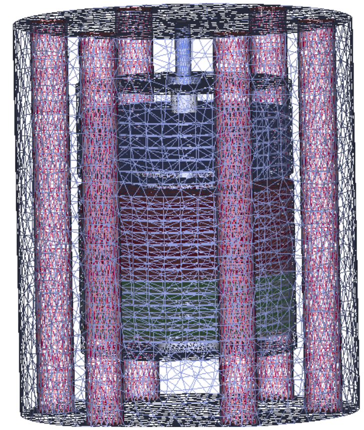
1754 Faces

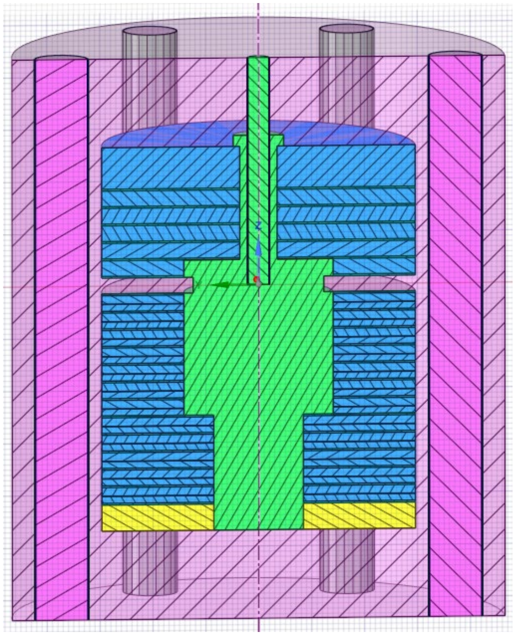
6880 Elements

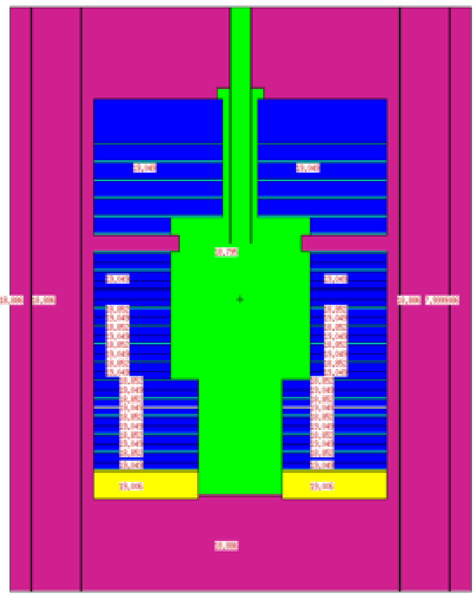


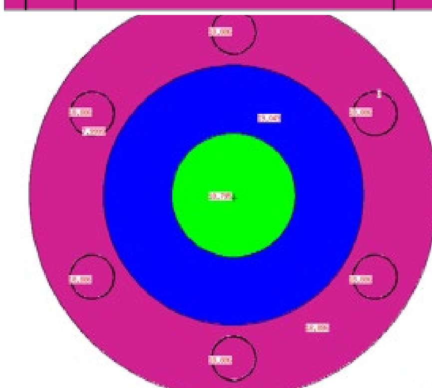
IMF007: Big Ten

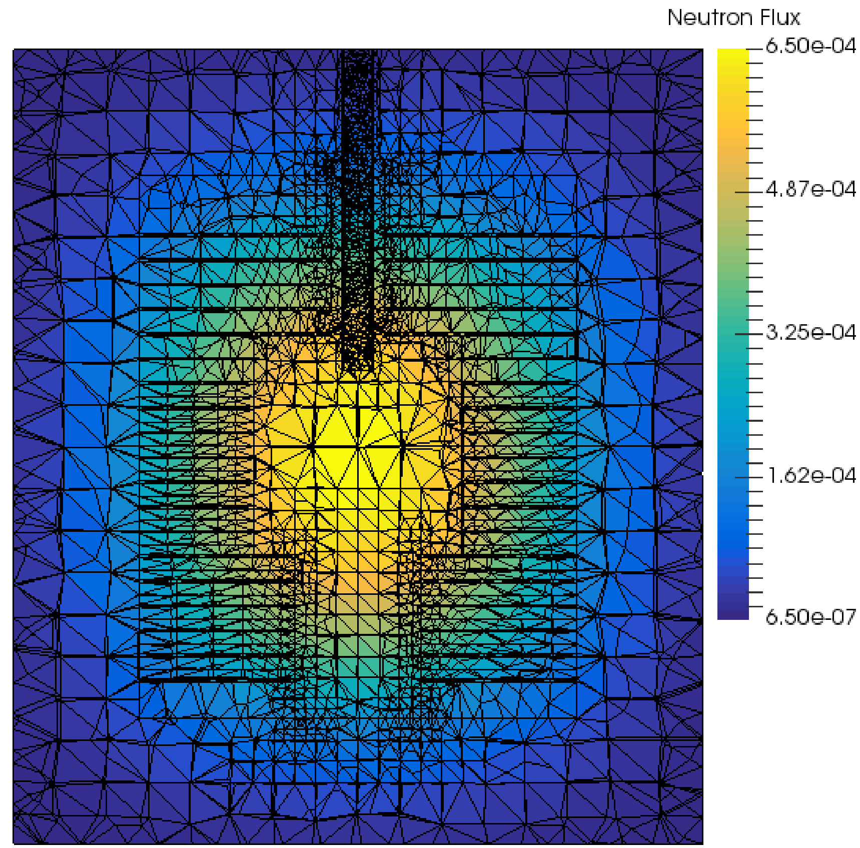
Benchmark	CSG % Diff	UM % Diff	C/E CSG	C/E UM
IEU-MET-FAST-007	-0.01%	-0.05%	0.9999	0.9995











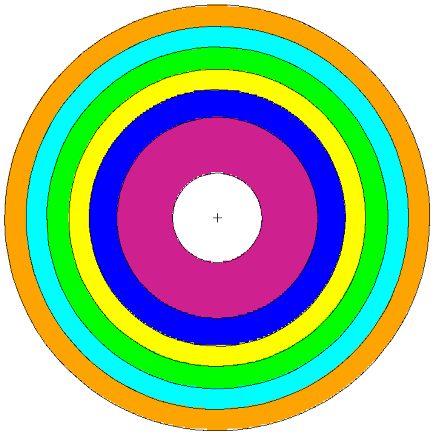
49,382 Nodes

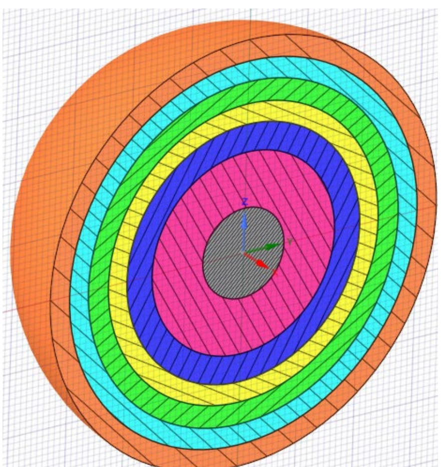
71,206 Faces

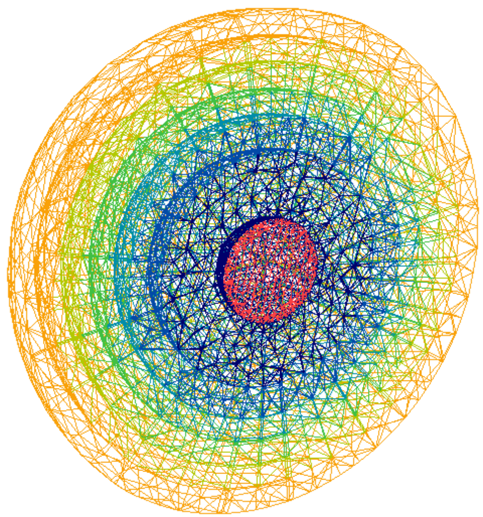
127,326 Elements

PMF022

Benchmark	CSG % Diff	UM % Diff	C/E CSG	C/E UM
PMF-022	-0.17%	-0.40%	0.9983	0.9960



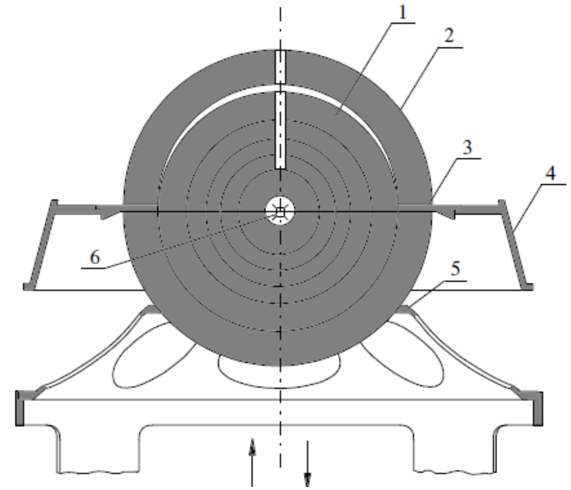


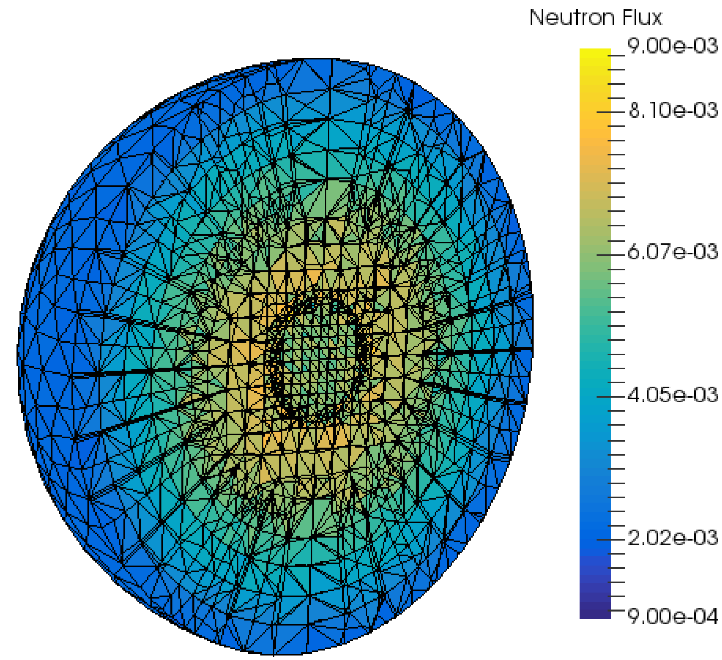


12,758 Nodes

10,496 Faces

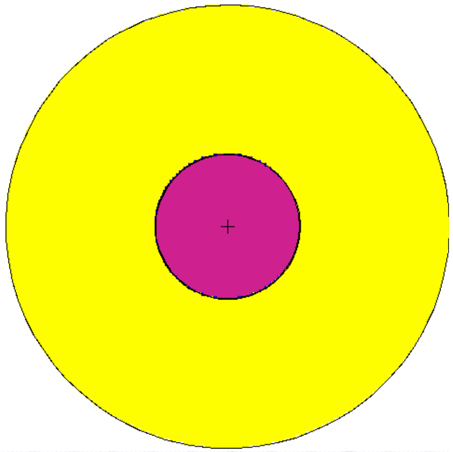
70,532 Elements

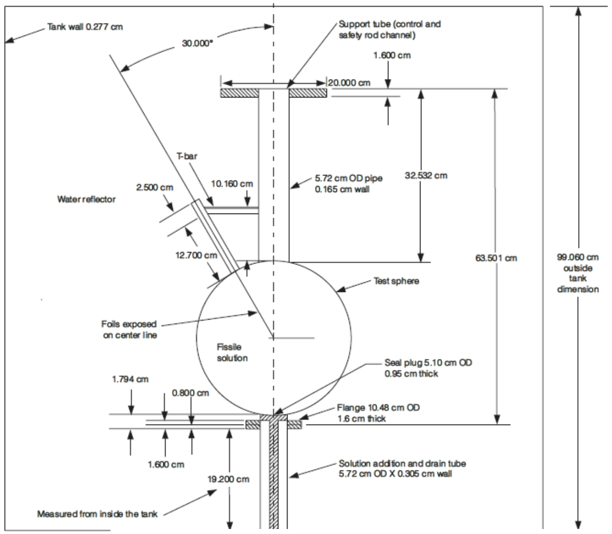


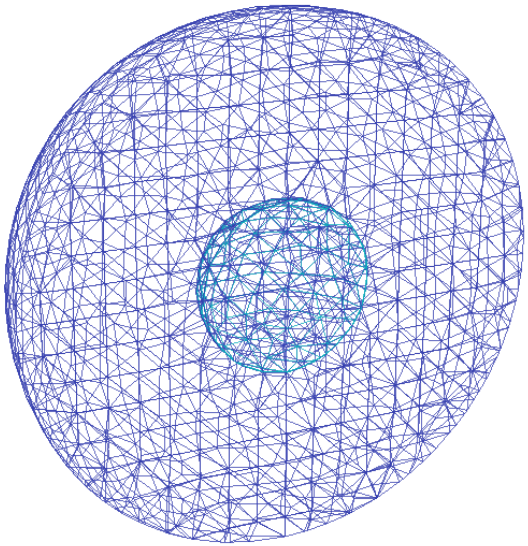


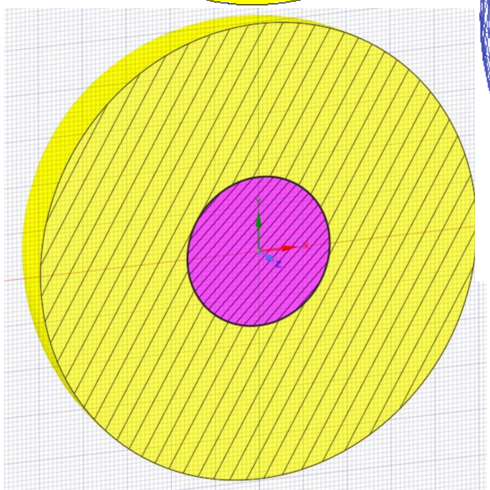
PST001

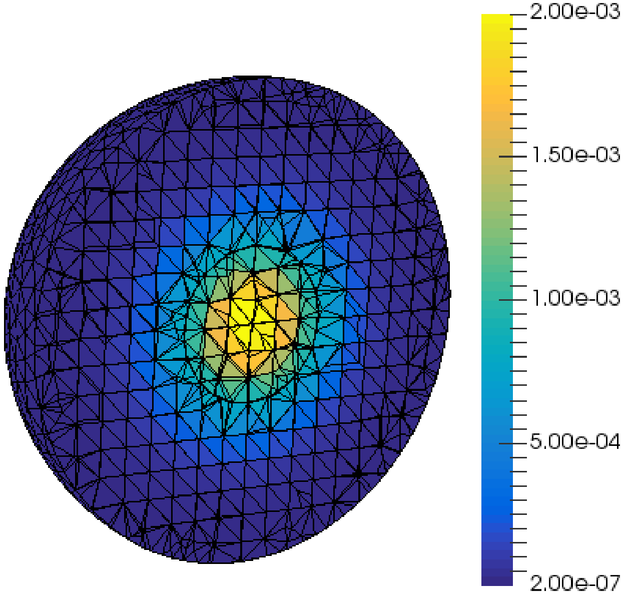
Benchmark	CSG % Diff	UM % Diff	C/E CSG	C/E UM
PST001-001	0.58%	0.30%	1.0058	1.0030









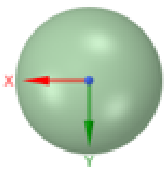


6,934 Nodes

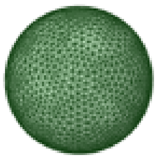
4,290 Faces

38,357 Elements

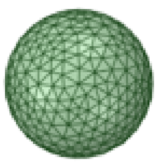
Mesh Technique: Max. Edge Length



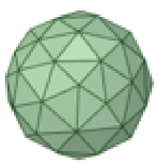
True Sphere (Radius = 8.741 cm)
Volume = 2797.4 cm³ | Area=960.1 cm²
SA/Vol = 0.343



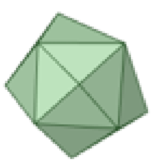
Meshed Sphere (Max Edge Length = 1 cm)
Volume = 2785.6 cm³ | Area = 957.6 cm²
SA/Vol = 0.344



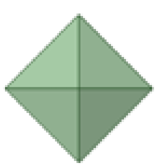
Meshed Sphere (Max Edge Length = 2 cm)
Volume = 2746.6 cm³ | Area = 950.3 cm²
SA/Vol = 0.346



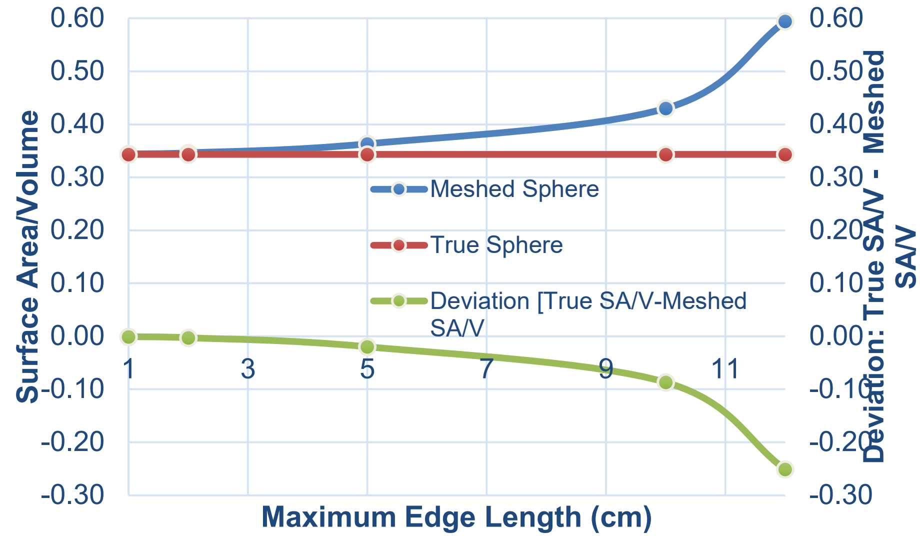
Meshed Sphere (Max Edge Length = 5 cm)
Volume=2480.9 cm³ | Area=899.2 cm²
SA/Vol = 0.363



Meshed Sphere (Max Edge Length = 10 cm)
Volume = 1748.3 cm³ | Area = 752.2 cm²
SA/Vol = 0.430

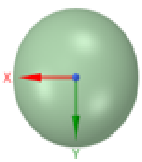


Meshed Sphere (Max Edge Length ≥ 12 cm)
Volume = 890.5 cm³ | Area = 529.2 cm²
SA/Vol = 0.594

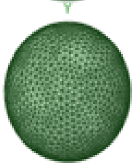


- *Mesh element size control: edge length*
  - Global, part-wise, feature based
  - Reduce edge length, increase elements
- *Edge length transition*
  - Interface between regions
  - Transition factor lowered for anisotropic curvature refinement

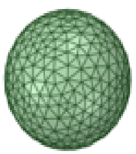
Mesh Technique: Density Adjustment



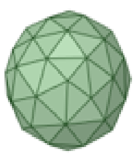
True Sphere (Radius = 8.741 cm)
Volume = 2797.4 cm^3 | Area=960.1 cm^2
SA/Vol = 0.343



Meshed Sphere (Max Edge Length = 1 cm)
Volume = 2785.6 cm^3 | Area = 957.6 cm^2
SA/Vol = 0.344



Meshed Sphere (Max Edge Length = 2 cm
Volume = 2746.6 cm^3 | Area = 950.3 cm^2
SA/Vol = 0.346



Meshed Sphere (Max Edge Length = 5 cm
Volume=2480.9 cm^3 | Area=899.2 cm^2
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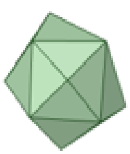

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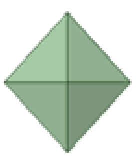

Meshed Sphere (Max Edge Length ≥ 12 cm)
Volume = 890.5 cm^3 | Area = 529.2 cm^2
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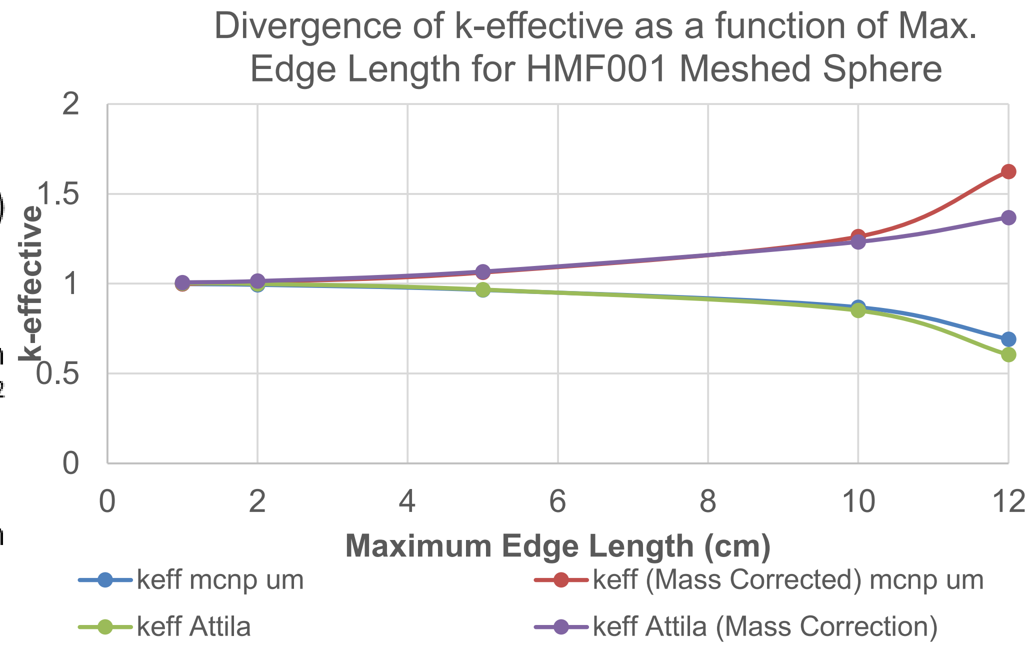
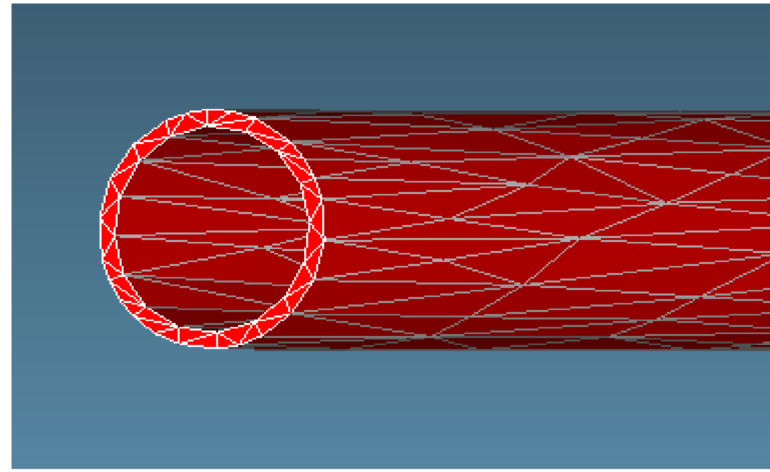


- Density Adjustment
  - by factor equal to ratio of true volume to mesh volume applied
  - For refinement of volumes within 2% and SA/V within 1%

Mesh Technique: Curvature Refinement

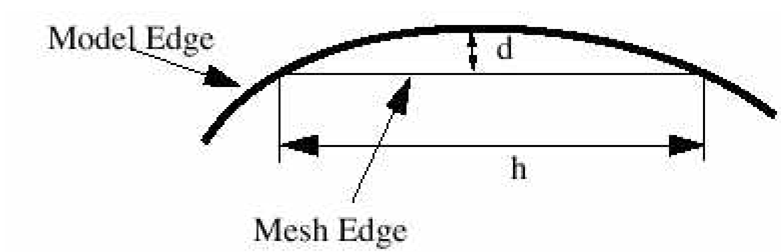
- Locally reduce element edge length to capture surface curvature
- Refine anisotropically: refine elements only in the curvature directions. Other directions determined by max edge length for that region

Anisotropic curvature refinement on annulus



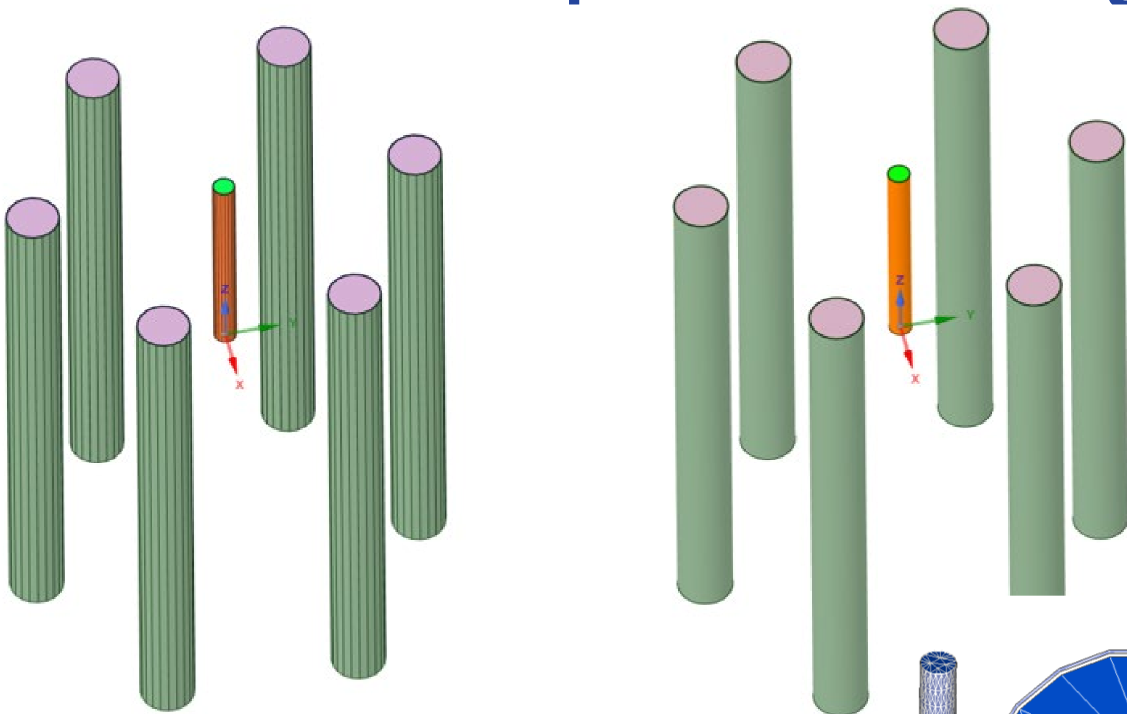
Curvature Refinement

Curvature refinement allows the mesh to be automatically refined to match the curvature of the entities in the geometric model. The mesh size is selected such that the distance of the model edge curve from the mesh edge (*d*) over the mesh edge length (*h*) **d/h** < 0.5. Useful values for **d/h** are typically in the range of 0.01 to 0.4 (smaller value = more refinement).



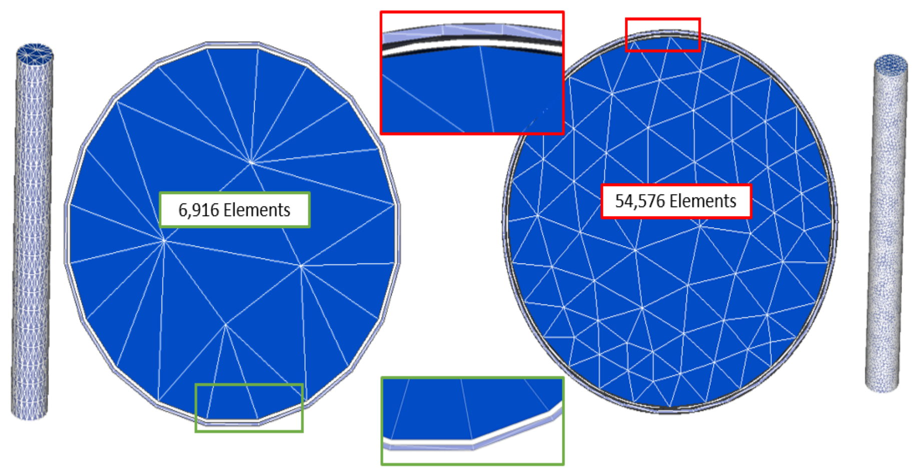
Ref.: Attila Training: Mesh Generation Process, Varex Imaging

Mesh Technique: Pre-faceting



20-sided polygon vs. true cylinder

- Radial tolerances strictly preserved
- Mesh size substantially reduced



Results/Conclusions

- It is possible to model critical benchmarks with MCNP6.2 UM to obtain k-effective results that are within one half of a percent of experimental values so long as due care is applied to mesh quality, especially in preserving both the mass and shape.

Benchmark	Experiment k-effective	Experiment uncertainty	MCNP6.2 CSG k-effective	MCNP6.2 CSG uncertainty	MCNP6.2 UM k-effective	MCNP6.2 UM uncertainty
HEU-MET-FAST-001	1.0000	0.10%	1.0000	0.01%	0.9984	0.01%
HEU-MET-FAST-007-037	0.9988	0.08%	1.0018	0.01%	1.0017	0.01%
IEU-MET-FAST-007	1.0045	0.07%	1.0044	0.01%	1.0040	0.01%
PU-MET-FAST-022	1.0000	0.21%	0.9983	0.01%	0.9960	0.06%
PU-SOL-THERM-001-001	1.0000	0.50%	1.0058	0.01%	1.0030	0.08%

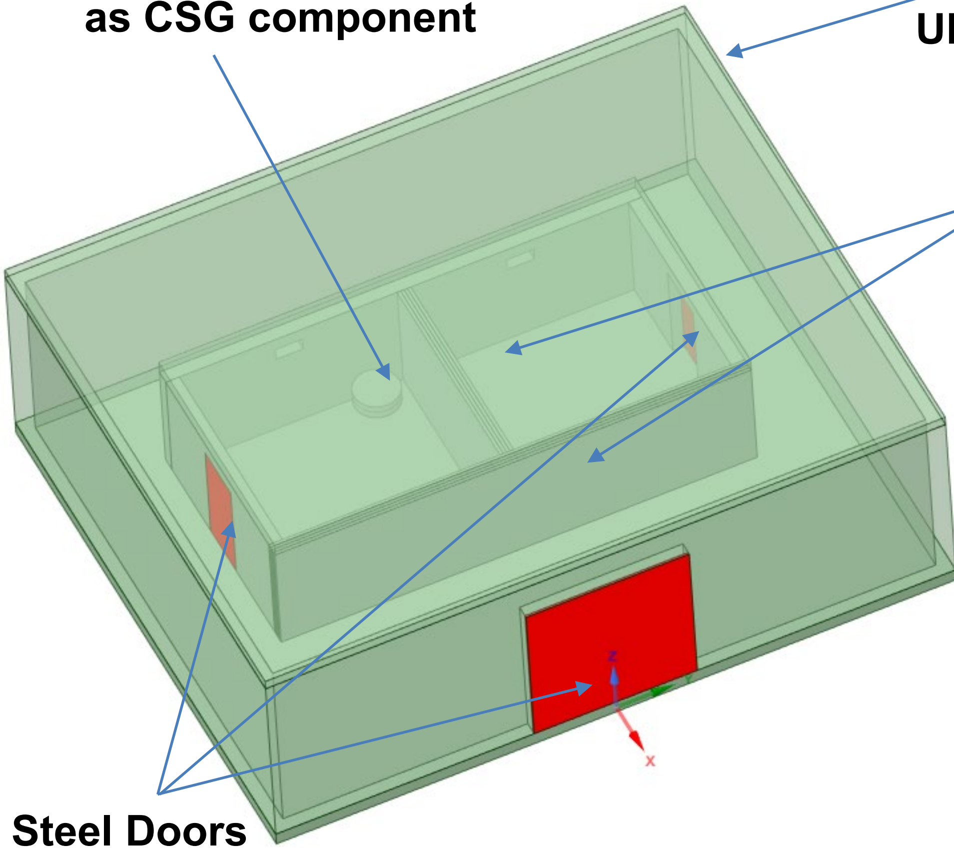
Benchmark	CSG % Diff	UM % Diff	C/E CSG	C/E UM
HEU-MET-FAST-001	0.00%	-0.16%	1.0000	0.9984
HEU-MET-FAST-007-037	0.30%	0.29%	1.0030	1.0029
IEU-MET-FAST-007	-0.01%	-0.05%	0.9999	0.9995
PU-MET-FAST-022	-0.17%	-0.40%	0.9983	0.9960
PU-SOL-THERM-001-001	0.58%	0.30%	1.0058	1.0030

CAAS CSG-UM Example

Critical assembly modeled as CSG component

Concrete Walls and Roof UM components

Spheres represent detectors modeled as CSG components



Steel Doors UM components