Los Alamos NATIONAL LABORATORY

Critical Benchmarks Modeled with MCNP® Unstructured Mesh

Nuclear Criticality Safety Program
Technical Program Review

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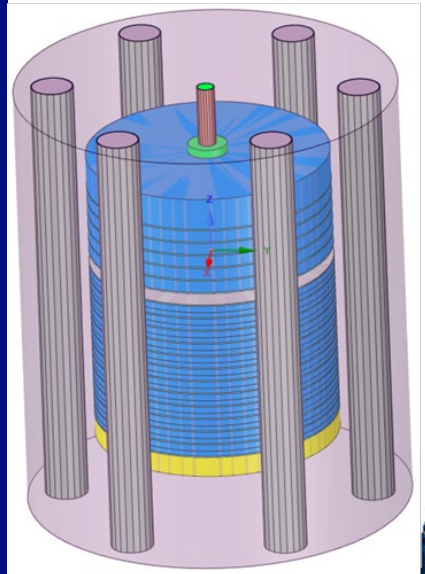
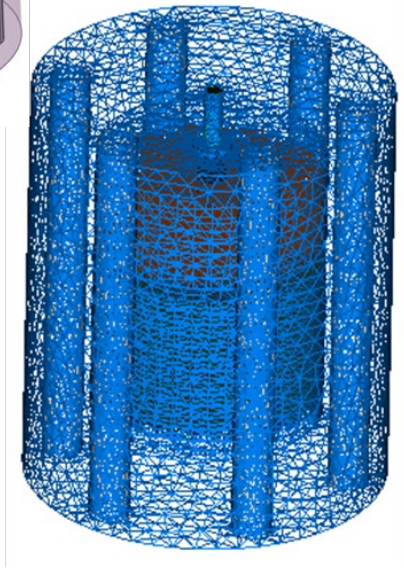
LA-UR-22-30840



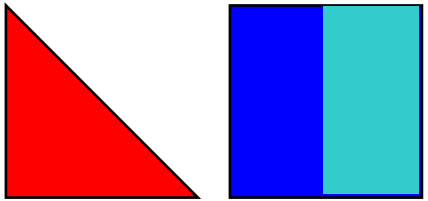


Unstructured Mesh Geometry

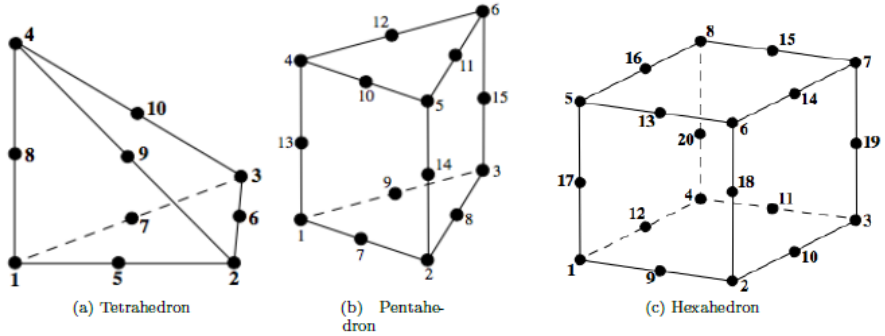
- Hybrid geometry in MCNP6
  - Capability to embed geometry representations such as structured and unstructured mesh (UM) within traditional constructive solid geometry (CSG) so that geometry representations work together
- MCNP UM development began 2006
  - Centered around LANL engineering capabilities using Abaqus
  - Abaqus formatted file with appropriately named element can be used in MCNP6
  - MCNP UM first released in MCNP6, bug fixes/new features in subsequent releases
- Calculation results tracked on the mesh & accumulated in special output file
  - MCNP6.3 - formatted as HDF5 file
- MCNP UM not yet widely adopted in NCS community

Unstructured Mesh Geometry

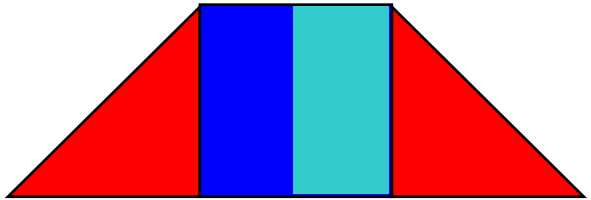
- MCNP UM geometry made up of elements (or “finite elements”) organized into parts that are instanced into an assembly.
- Elements may be 1st or 2nd order tetrahedra, pentahedral, hexahedra, or continuum shell element



parts



elements

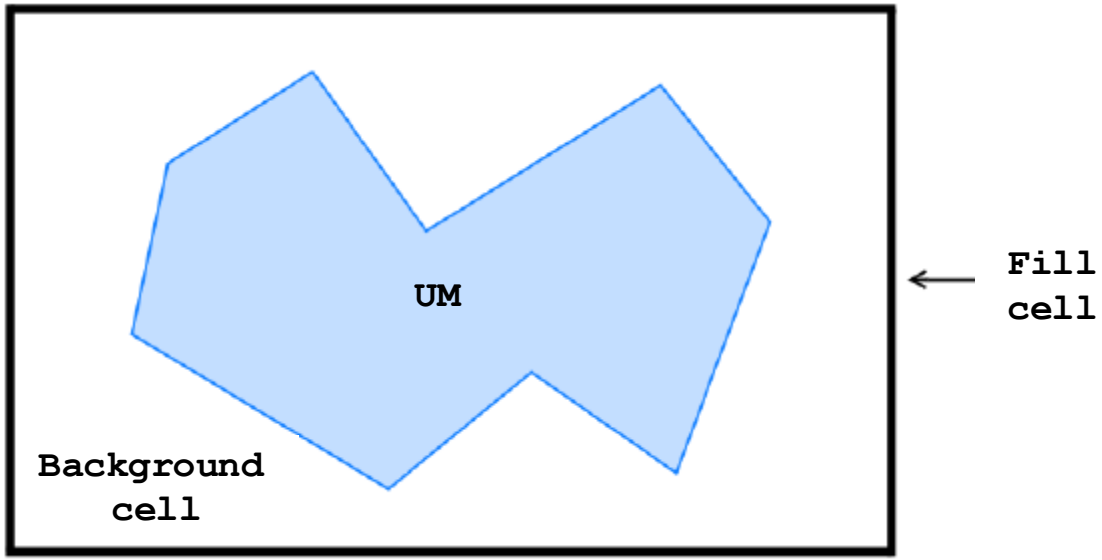


assembly

2 instances of red part
1 instance of blue-green part

Unstructured Mesh Geometry

- Computer aided engineering (CAE) or computer aided design (CAD) tools can be used to create a 3-dimensional model
- The solid model can be meshed into an UM representation
- The UM representation can coexist with other geometry types in MCNP

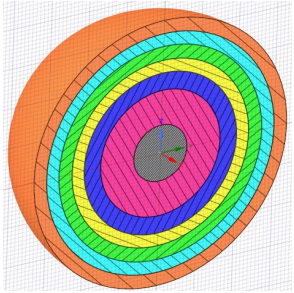


Criticality Calculations with UM Geometry

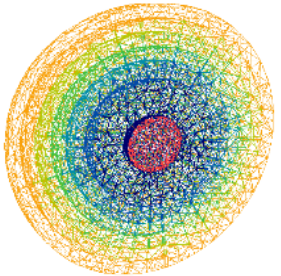
- Mesh Quality is important
  - Mass/volume may not be preserved
  - Especially important for criticality calculations
  - Goal - preserve volume to the degree necessary for correct criticality calculation, finer mesh (true volume) vs. coarser mesh (reduced computational time)
- **Ongoing work to assess criticality calculations with MCNP UM**
- MCNP UM k-effective results are ≈ 0.5 % experimental benchmark values with due care is applied to mesh quality, preserving both the mass and shape
- Pre- and post-MCNP-calculation mesh interrogation methods and UM quality assessment checks available [1]
  - Including visualization of mesh quality

Criticality Calculations with UM Geometry

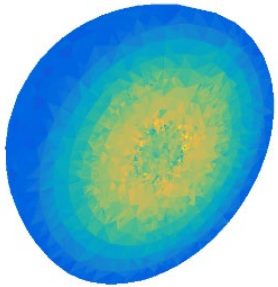
1. Construct solid geometry (SpaceClaim [9])
2. Create mesh of solid geometry in abaqus formatted file
   - Attila4MC [10], Abaqus [11], CUBIT [12], or similar package
   - Study uses 1st order tetrahedral elements;
   - 2nd order elements may be efficient with regard to curvature
3. Create MCNP6 input file & modify to specify kcode parameters
4. Execute MCNP6 kcode, pass statistical & convergence checks
5. Compare calculated k-effective result with experiment result [8]
   (UM results are comparable to CSG results)
6. Visualize MCNP6 results (Paraview [13,14])



SpaceClaim



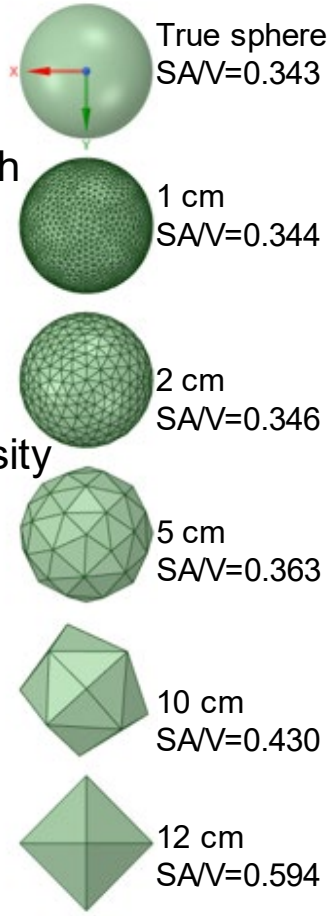
Attila4MC Mesh

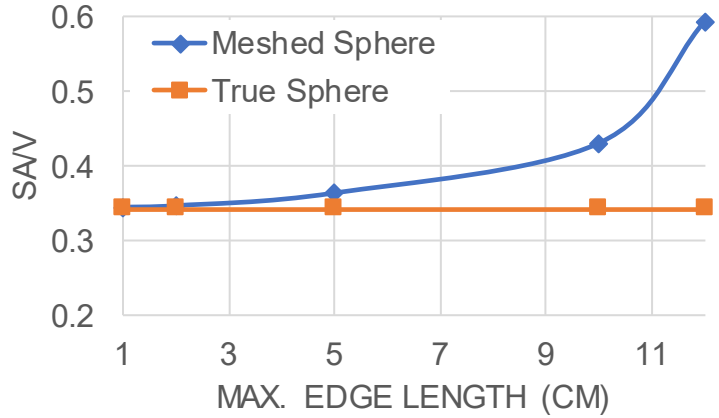


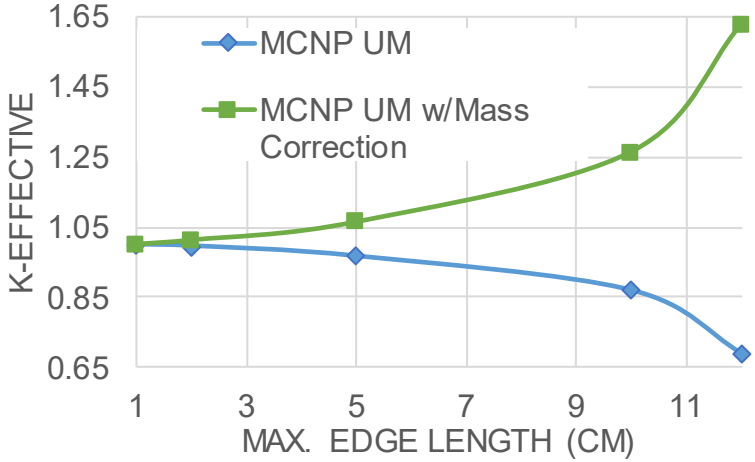
Paraview

Mesh Techniques

- Element size control
  - Set when creating mesh
  - Recommend
    - Δ Volume ≤ 2%,
    - Δ SA/V ≤ 1%
- Mass correction
  - Factor applied to density based upon vol_{true}/vol_{meshed}

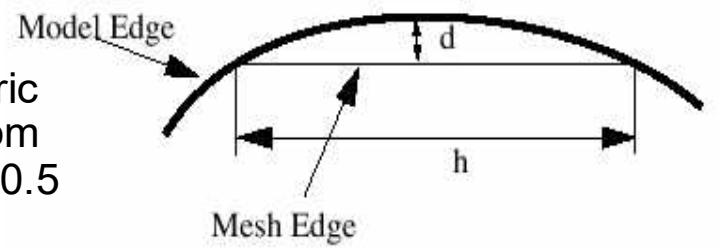




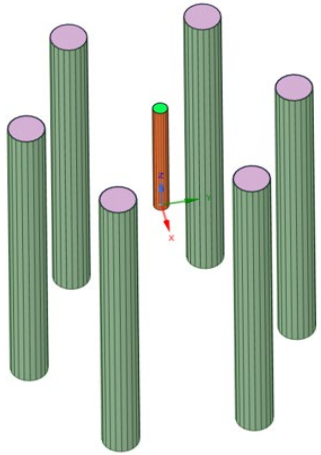


Mesh Techniques

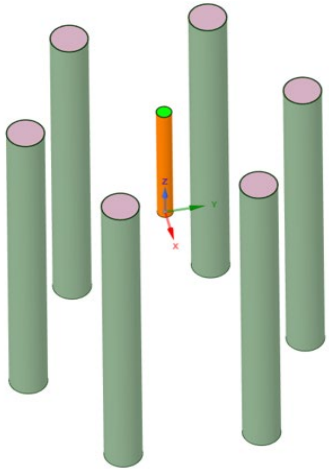
- Curvature refinement [10]
  - Refine mesh to match curvature of geometric model such that distance of model edge from mesh edge, d, over mesh edge length, h < 0.5



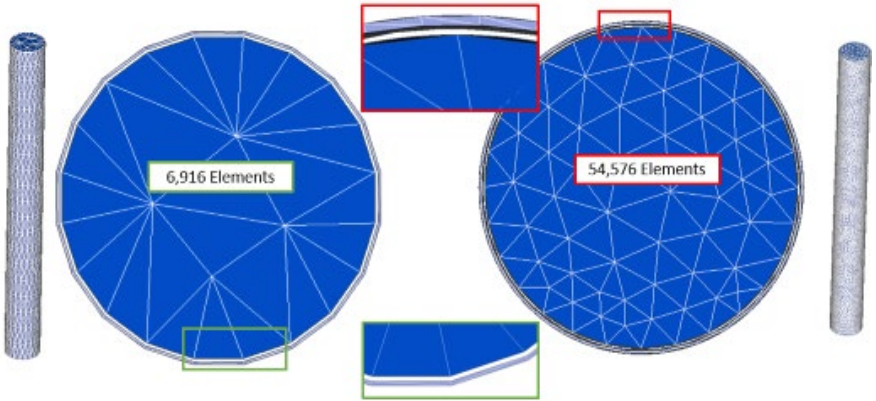
- Pre-faceting



20-sided Polygon



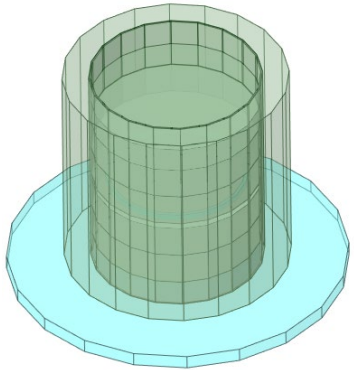
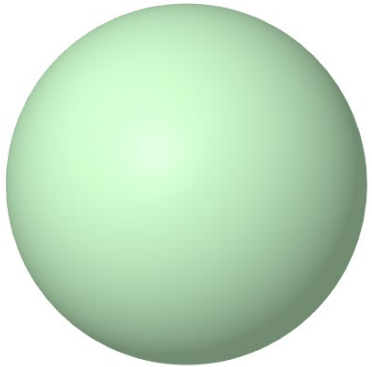
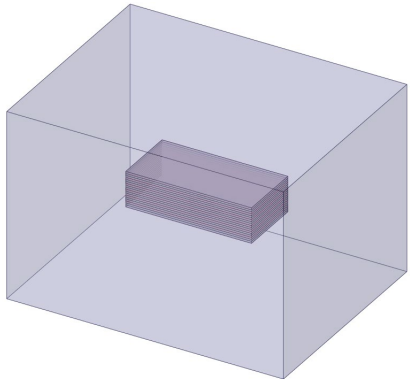
True Cylinder



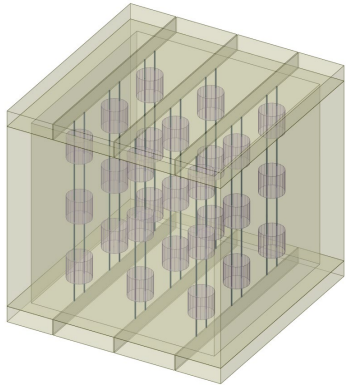
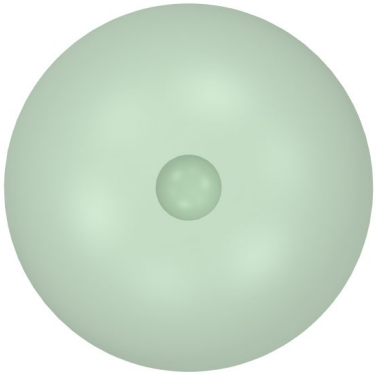
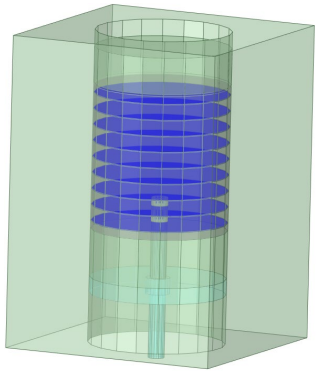
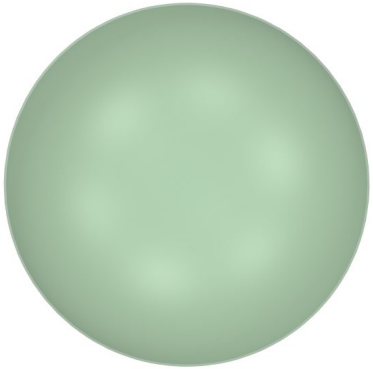
20-sided Polygon

True Cylinder

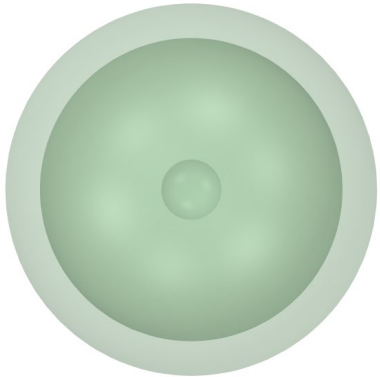
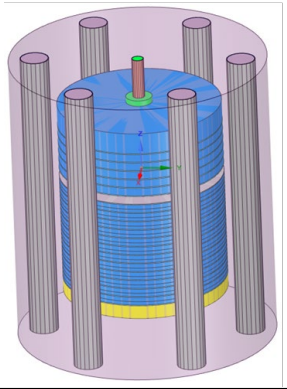
Benchmark Results

	HCI-003-006	HMF-001	HMF-004	HMF-007-037
				
	UH_3 cylinders reflected by DU	Godiva – bare, fast, sphere of HEU metal	HEU sphere reflected by water	HEU metal slabs, polyethylene moderated & reflected
MCNP6	0.994934 ± 0.000497	0.998755 ± 0.000084	0.996882 ± 0.00011	1.001650 ± 0.000116
Exp.	1.0000 ± 0.0047	1.000 ± 0.001	1.0020	0.9988 ± 0.0008
C/E	0.9949	0.9987	0.9949	1.0028

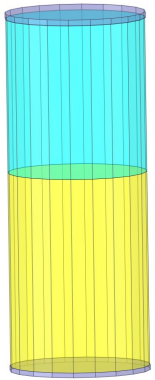
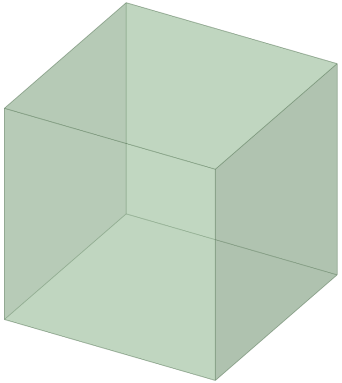
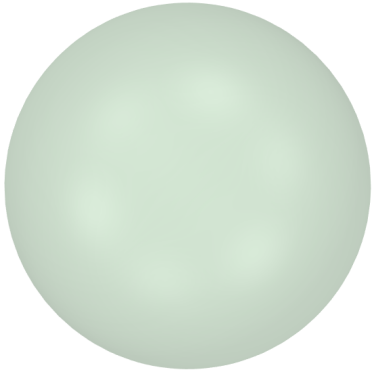
Benchmark Results

	HMF-026-021	HMF-028	HMI-006-002	HST-032
				
	3 x 3 x 3 array of HEU cylinders in paraffin box	HEU sphere reflected by NU	HEU platters moderated by graphite, reflected by copper	Bare sphere of HEU nitrate solution
MCNP6	1.003254 ± 0.000114	1.004913 ± 0.000094	0.999191 ± 0.000106	0.998717 ± 0.000055
Exp.	1.0000 ± 0.0038	1.0000 ± 0.0030	1.0001 ± 0.0008	1.0015 ± 0.0026
C/E	1.0032	1.0049	0.9991	0.9972

Benchmark Results

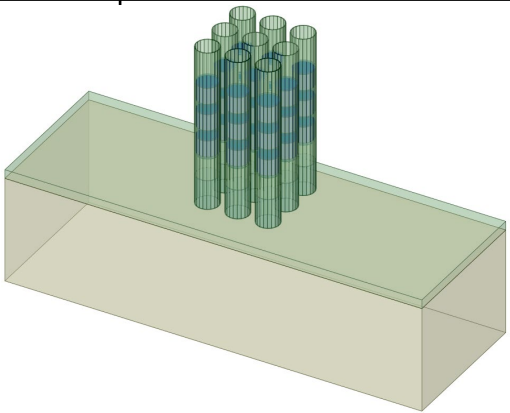
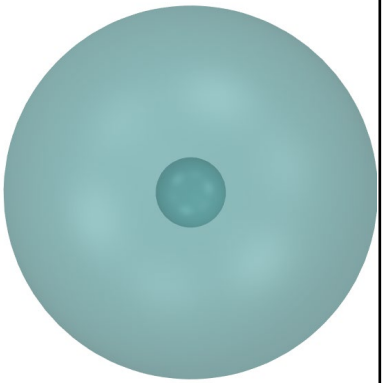
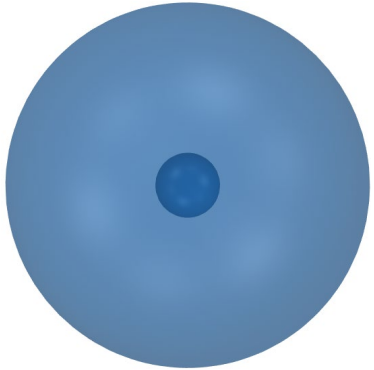
	IMF-003	IMF-004	IMF-007	LST-002-002
				
	Bare sphere of IEU (36 wt% ^{235}U)	Sphere of IEU reflected by graphite (36 wt% ^{235}U)	Big Ten, cylindrical core ~10% avg ^{235}U enrichment, thick ^{238}U reflector	Bare sphere of LEU (4.9 wt% ^{235}U) uranyl fluoride solution
MCNP6	0.999117 ± 0.000091	1.004915 ± 0.000087	1.00366 ± 0.00026	0.996070 ± 0.000091
Exp.	1.0000 ± 0.0019	1.0000 ± 0.0032	1.0045 ± 0.0007	1.0024 ± 0.0037
C/E	0.9991	1.0049	0.9992	0.9961

Benchmark Results

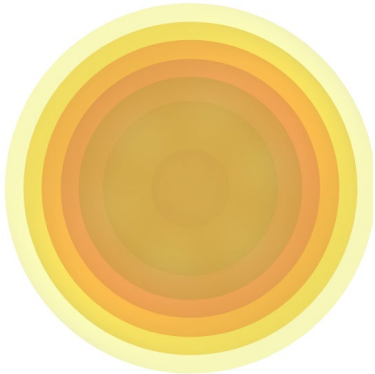
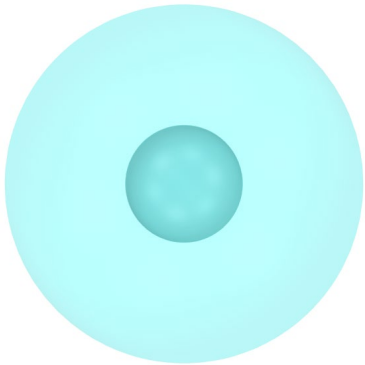
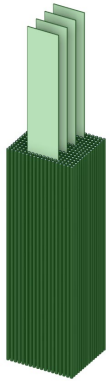
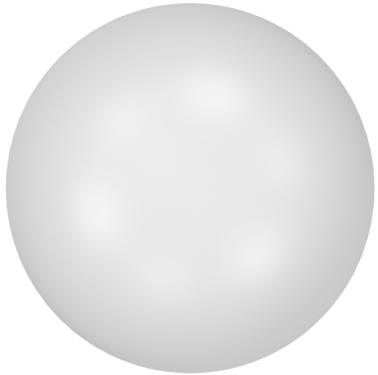
	LST-007-036	PCI-001-001	PMF-001	PMF-002
				
	Cylindrical tank of uranyl nitrate solution	Homogenous mixture of Pu, hydrogen, and graphite	Bare sphere of ^{239}Pu metal	Bare sphere of Pu metal, ~20% ^{240}Pu
MCNP6	0.998784 ± 0.000090	1.011829* ± 0.000507	0.999959 ± 0.000303	1.000618 ± 0.000086
Exp.	0.9988 ± 0.0011	1.0000 ± 0.0110	1.00000 ± 0.00110	1.000 ± 0.002
C/E	1.0000	1.0118	0.9999	1.0006

*PCI-001-001 CSG Model also calculates high, k-eff = 1.01174 ± 0.00007

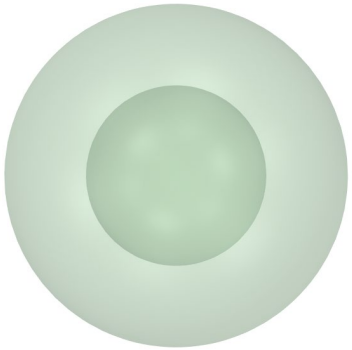
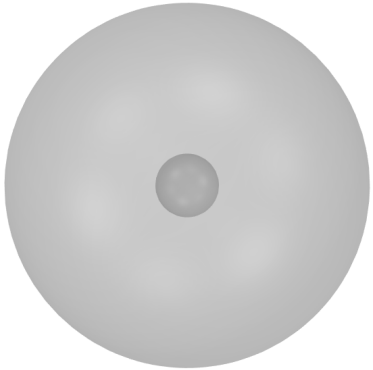
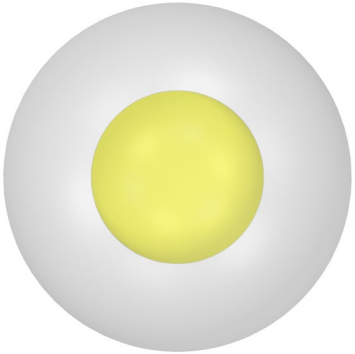
Benchmark Results

	PMF-003-103	PMF-006	PMF-008	PMF-011
				
	3 x 3 x 3 array of small cylinders of Pu	Pu sphere reflected by NU	Pu sphere reflected by Th	Pu sphere reflected by water
MCNP6	1.002000 ± 0.000760	0.998429 ± 0.000096	0.995053 ± 0.000494	0.994325 ± 0.000108
Exp.	1.00 ± 0.003	1.0000 ± 0.0030	1.000 ± 0.0006	1.000 ± 0.001
C/E	1.0020	0.9984	0.9951	0.9942

Benchmark Results

	PMF-022	PST-001	UCT-001-003	UMF-001
				
	Bare, fast, spherical assembly of Pu shells	Water-reflected 11.5-inch diameter sphere of Pu nitrate solution	Lattice of ^{233}U fuel pins in water	Bare sphere of ^{233}U
MCNP6	0.996265 ± 0.000082	0.997380 ± 0.000877	1.006317 ± 0.000800	0.999870 ± 0.000076
Exp.	1.0000 ± 0.0021	1.0000 ± 0.0050	1.0000 ± 0.0024	1.000 ± 0.001
C/E	0.9963	1.0030	1.0063	0.9990

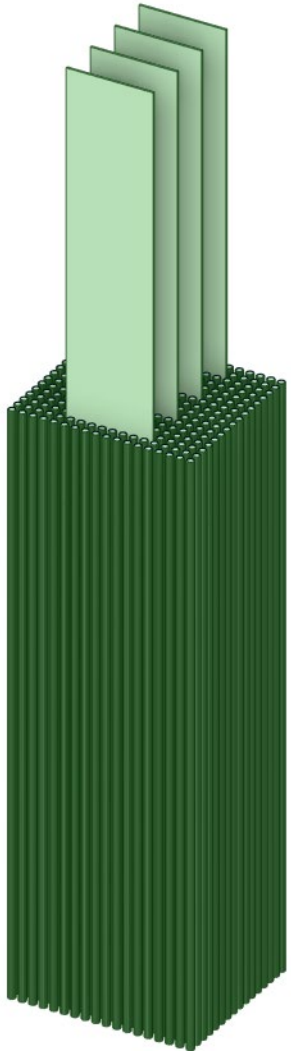
Benchmark Results

	UMF-005-002	UMF-006	USI-001-001	UST-008
				
	Sphere of ^{233}U reflected by Be	Sphere of ^{233U} reflected by NU	Be-reflected sphere of uranyl fluoride solution enriched in ^{233}U	Sphere of uranyl fluoride solution enriched in ^{233}U
MCNP6	0.994000 ± 0.000099	0.998510 ± 0.000099	0.985362* ± 0.000667	1.000040 ± 0.000052
Exp.	1.0000 ± 0.0030	1.0000 ± 0.0014	1.0000 ± 0.0083	1.0006 ± 0.0029
C/E	0.9940	0.9985	0.9854	0.9998

*USI-001-001 CSG Model also calculates low, k-eff = 0.98507 ± 0.00016

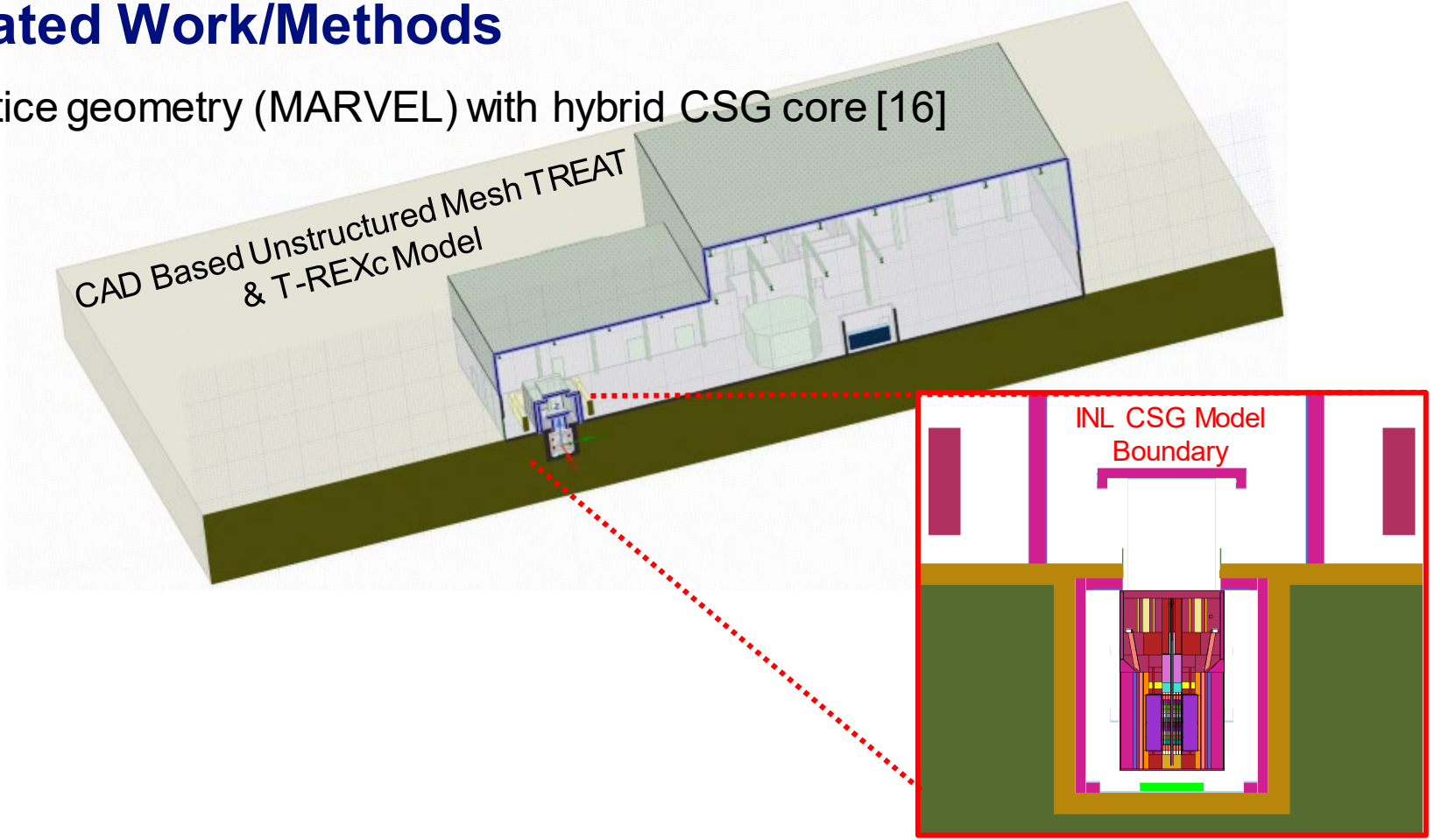
Results/Continuing Work

- Work in progress
  - Critical benchmarks using MCNP UM being studied
  - Testing and comparisons of mesh and MCNP6.3 options
  - Determine review process and file types in repository
  - Open-source git repository and release process
  - Most results within ~ ½ % of experiment
  - Computer time 10-40x CSG
    - HMF1 UM walltime ~50 min. for 5e7 neutrons on HPC
    - UCT1 UM walltime ~30 min. for 1e6 neutrons on HPC
  - Discussions with SNL for collaboration
- Lessons learned
  - Lattice geometry inside CSG water tank (UCI-001-003)
  - Lattice geometry (MARVEL) with hybrid CSG core [16]



Related Work/Methods

- Lattice geometry (MARVEL) with hybrid CSG core [16]



References

[1] J. A. Kulesza, "MCNP Unstructured Mesh Elemental Quality Assessment," Tech. Rep. LA-UR-21-26362, Los Alamos National Laboratory, Los Alamos, NM, USA, July 2021.

[2] C. J. Stimpson, C. D. Ernst, P. K. and. P. P. Pébay, and D. Thompson, "The Verdict Geometric Quality Library," Tech. Rep. SAND2007-1751, Sandia National Laboratories, Albuquerque, NM, USA, Mar. 2007.

[3] J. A. Kulesza, "MCNP® Code Version 6.3.0 Unstructured-mesh Quality Metrics & Assessment," Tech. Rep. LA-UR-20-27150 (rev.1), Los Alamos National Laboratory, Los Alamos, NM, USA, Sept. 2022. doi:10.2172/1888190.

[4] P. M. Knupp, "Achieving Finite Element Mesh Quality Via Optimization of the Jacobian Matrix Norm and Associated Quantities. Part II—A Framework for Volume Mesh Optimization and the Condition Number of the Jacobian Matrix," International Journal for Numerical Methods in Engineering, vol. 48, pp. 1165–1185, May 2000.

[5] P. M. Knupp, "Algebraic Mesh Quality Metrics for Unstructured Initial Meshes," Finite Elements in Analysis and Design, vol. 39, pp. 217–241, Jan. 2003.

[6] P. P. Pébay, D. Thompson, J. Shepherd, P. Knupp, C. Lisle, V. A. Magnotta,and N. M. Grosland, "New Applications of the Verdict Library for Standardized Mesh Verification Pre, Post, and End-to-End Processing," in Proceedings of the 16th International Meshing Roundtable (M. L. Brewer and D. Marcum, eds.), (Seattle, WA, USA; October 15–17), pp. 535–552, 2008.

[7] J. A. Kulesza, T. R. Adams, J. C. Armstrong, S. R. Bolding, F. B. Brown, J. S. Bull, T. P. Burke, A. R. Clark, R. A. Forster III, J. F. Giron, A. S. Grieve, C. J. Josey, R. L. Martz, G. W. McKinney, E. J. Pearson, M. E. Rising, C. J. Solomon Jr., S. Swaminarayan, T. J. Trahan, S. C. Wilson, and A. J. Zukaitis. MCNP® Code Version 6.3.0 Theory & User Manual. Los Alamos National Laboratory Tech. Rep. LA-UR-22-30006, Rev. 1. Los Alamos, NM, USA. 2022. https://mcnp.lanl.gov/manual.html

References

[8] International Handbook of Evaluated Criticality Safety Benchmark Experiments, NEA/NSC/DOC(95)03/I, Volume I, 2020 edition.

[9] SpaceClaim. ANSYS SpaceClaim, www.spaceclaim.com

[10] Attila4MC, Silver Fir Software, https://silverfirsoftware.com/

[11] Abaqus. Dassault Systems. Abaqus Unified FEA. www.3ds.com/products-services/similia/products/abaqus

[12] CUBIT, Sandia National Laboratories, https://cubit.sandia.gov/

[13] J. A. Kulesza, T. C. McClanahan. 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 (rev.1). 2019.

[14] The Paraview Guide, Kitware, Inc, www.Paraview.org/Paraview-guide

[15] J. Wagner, E. Blakeman, and D. Peplow, “Forward-Weighted CADIS Method for Variance Reduction of Monte Carlo Calculations of Distributions and Multiple Localized Quantities”. *International Conference on Mathematics, Computational Methods & Reactor Physics*, Saratoga Springs, NY (2009).

[16] J. Spencer, H. Trellue, T. Lange, T. Funderburg, MARVEL Reactor Shield Design. Los Alamos National Laboratory, LA-UR-22-29101 . 2022.

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