LA-UR-21-25913
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Title: Utilizing Unstructured Mesh Geometry in Criticality Calculations and Criticality Accident Alarm System Analysis

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Intended for: MCNP Users Symposium, 2021-07-12 (Los Alamas, New Mexico, United States)

Issued: 2021-06-23

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Utilizing Unstructured Mesh Geometry in Criticality Calculations and Criticality Accident Alarm System Analysis

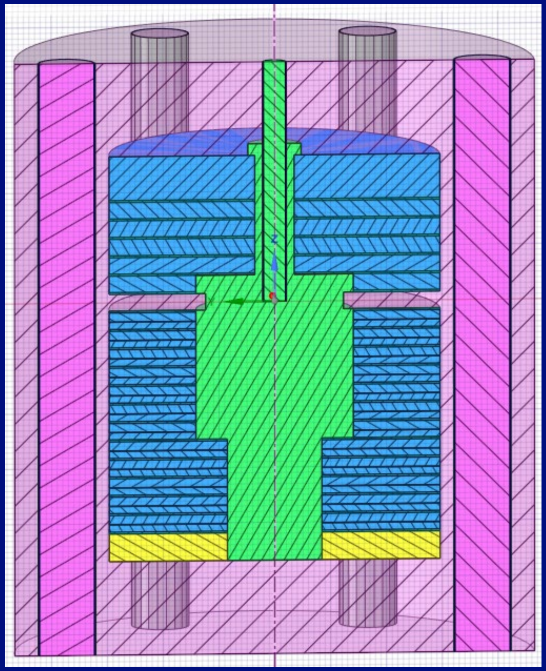
J.L. Alwin, J.B. Spencer

12 July 2021

Presentation Topics

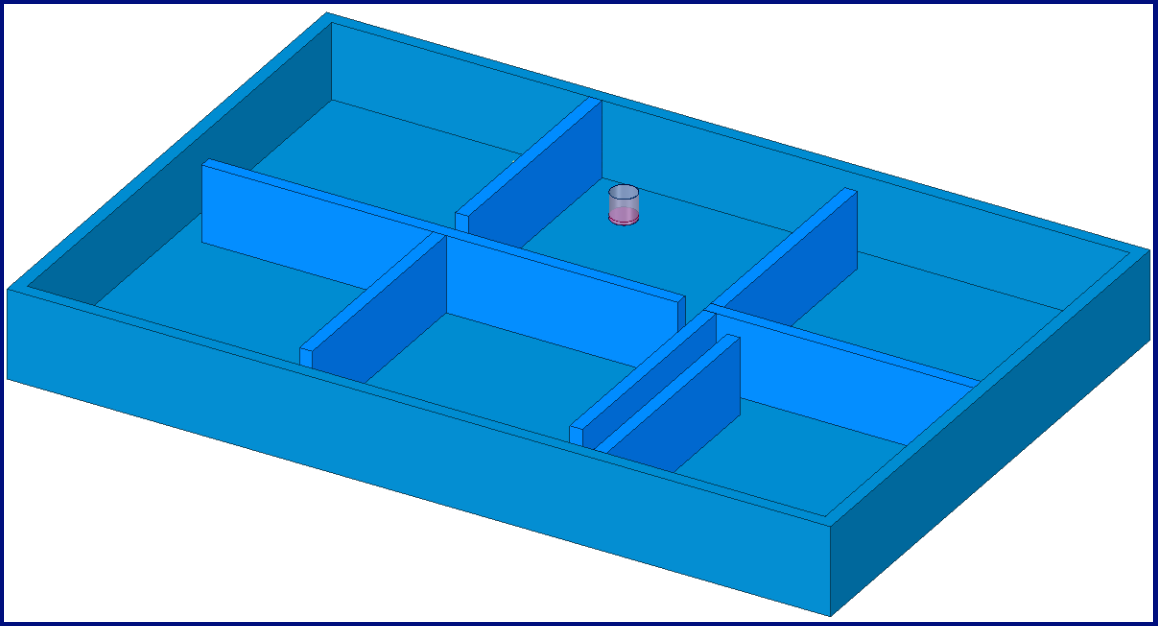
Criticality Calculations

- MCNP6.2 Results Compared with Experiments
  - Constructive Solid Geometry (CSG)
  - Unstructured Mesh (UM)

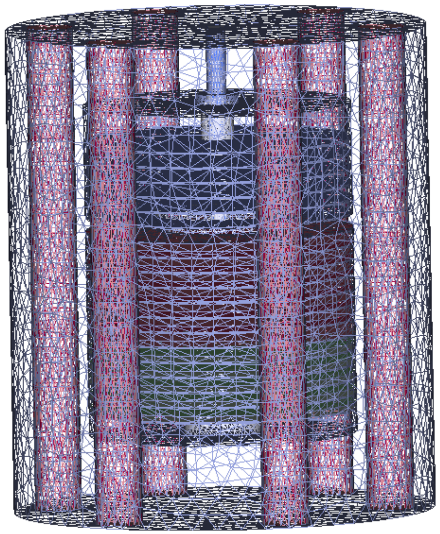


Criticality Accident Alarm System (CAAS) Analysis

- MCNP6.2 Results using Hybrid Geometry & Variance Reduction
  - CSG combined with UM Geometry
  - Weight Windows via Deterministic method used in MCNP6.2



Criticality Calculations with UM Geometry



Mesh Quality is important

- Mass/volume may not be preserved
- Especially important for criticality calculations

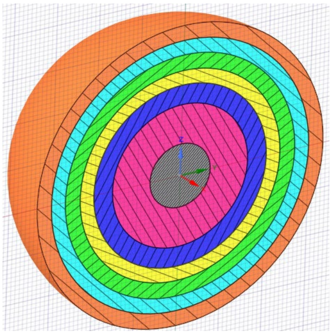
- It is possible to generate a mesh, which reflects the geometry adequately for most purposes, and yet does not properly preserve mass and/or volume to the degree necessary for correct criticality calculation leading to incorrect k-effective results

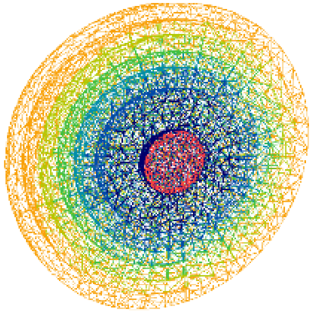
In this work, results of a set of criticality calculations with MCNP UM are successful →

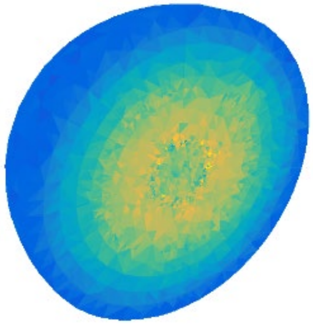
- Critical benchmarks with MCNP6.2 UM k-effective results that are ≈ ½% experimental values **when due care is applied to mesh quality**, in preserving both the mass and shape.

Critical Benchmarks using MCNP6.2 UM Geometry

- **HEU-MET-FAST-001**: Godiva- bare, fast, spherical assembly of ^{235}U metal.
- **HEU-MET-FAST-007-037**: HEU metal slabs, polyethylene moderated & reflected.
- **IEU-MET-FAST-007**: Big Ten- 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.





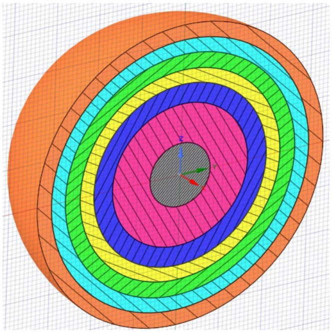


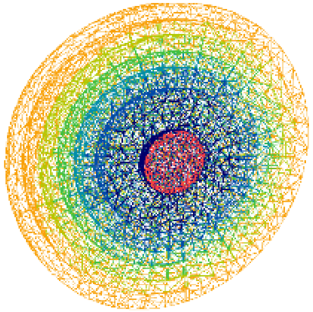
Determine engineering best practices for mesh parameters

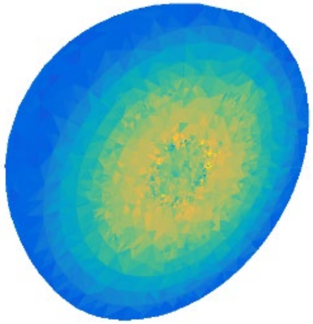
- Mesh within mass and/or volume tolerances →1-2%
  - Volume within 2%, SA/V within 1%, density adjustment refinement
- Provide description of expert techniques
- Compare MCNP6.2 results and experiment results → bias ≈ ½%

Critical Benchmarks using MCNP6.2 UM Geometry

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





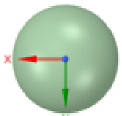


- May use Abaqus[5] directly. Study uses Attila4MC to generate Abaqus file, engi practices offered apply equally well, regardless of model construction method.
- Study uses 1st order tetrahedral elements, 2nd order elements may be efficient curvature, the same engineering best practices apply

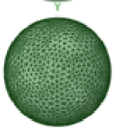
1. SpaceClaim. ANSYS SpaceClaim, www.spaceclaim.com
2. 2. Attila4MC, Silver Fir Software, https://silverfirsoftware.com/
3. 3. Kulesza, Joel. A Python Script to Convert MCNP Unstructured Mesh Elemental Edit Output Files to XML-based VTK Files. Los Alamos National Laboratory, LA-UR-19-20291. 2019.
4.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

HEU-MET-FAST-001 Godiva

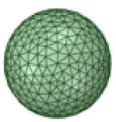
- Mesh Technique: Element Size Control



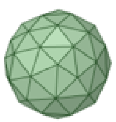
True Sphere (Radius = 8.741 cm)
Volume = 2797.4 cm^3 | Area=960.1 cm^2
SA/Vol = 0.343



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

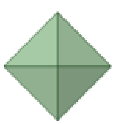


Meshed Sphere (Max Edge Length = 2 cm)
Volume = 2746.6 cm^3 | Area = 950.3 cm^2
SA/Vol = 0.346

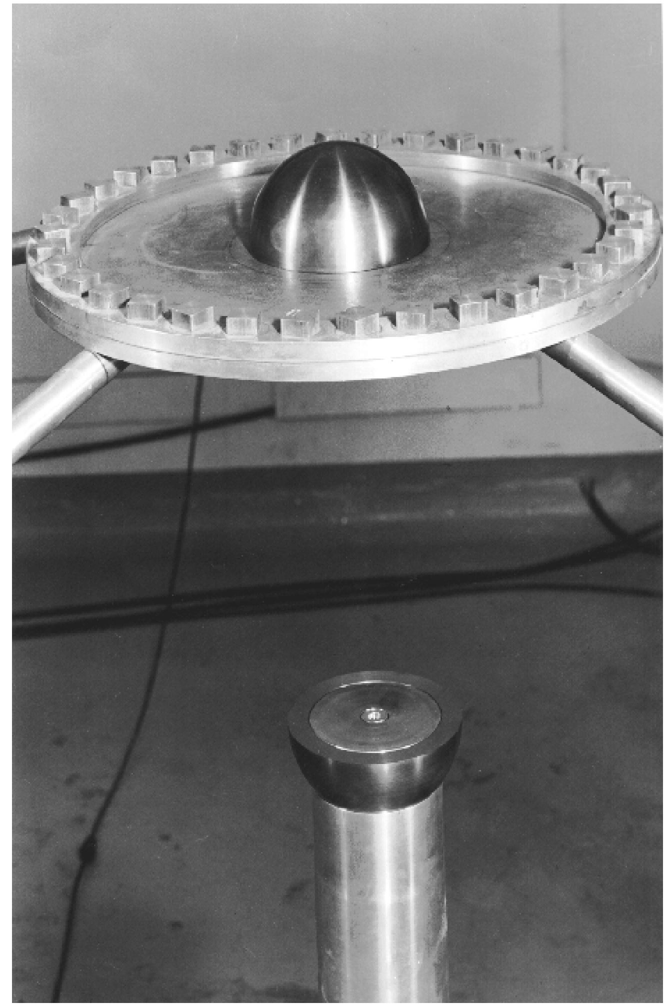


Meshed Sphere (Max Edge Length = 5 cm)
Volume=2480.9 cm^3 | Area=899.2 cm^2
SA/Vol = 0.363

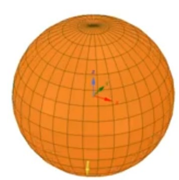
Meshed Sphere (Max Edge Length = 10 cm)
Volume = 1748.3 cm^3 | Area = 752.2 cm^2
SA/Vol = 0.430



Meshed Sphere (Max Edge Length ≥ 12 cm)
Volume = 890.5 cm^3 | Area = 529.2 cm^2
SA/Vol = 0.594

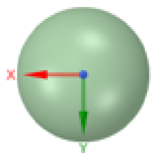


- Mesh Technique: Mass Correction
  - Apply factor to density based upon Vol_{true}/Vol_{meshed}
- Mesh Technique: Tessellated Body
  - Convert sphere to tessellated body[1] in SpaceClaim:



HEU-MET-FAST-001 Godiva

- Mesh Technique:
- Element Size Control & Mass Correction



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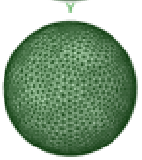

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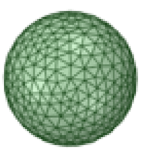

Meshed Sphere (Max Edge Length = 2 cm)
Volume = 2746.6 cm^3 | Area = 950.3 cm^2
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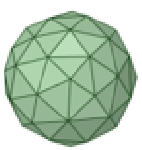

Meshed Sphere (Max Edge Length = 5 cm)
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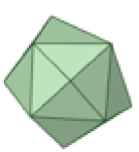

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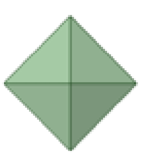
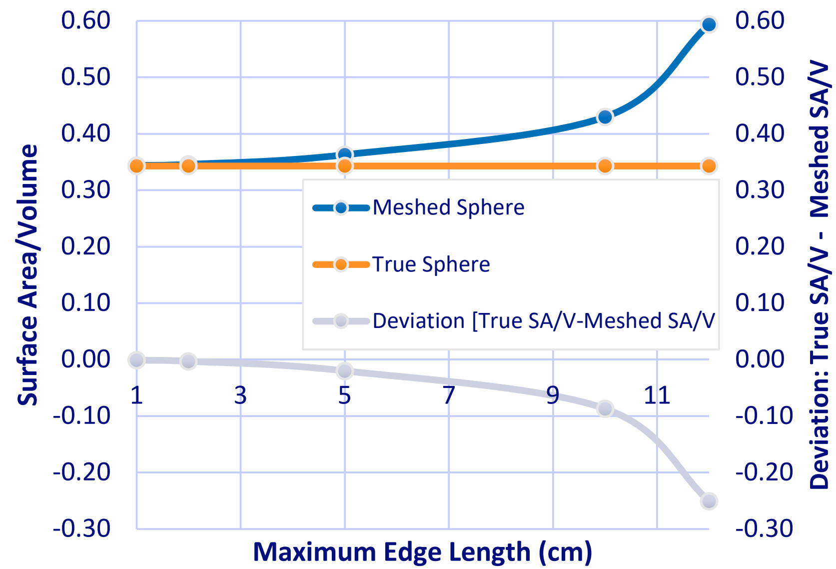
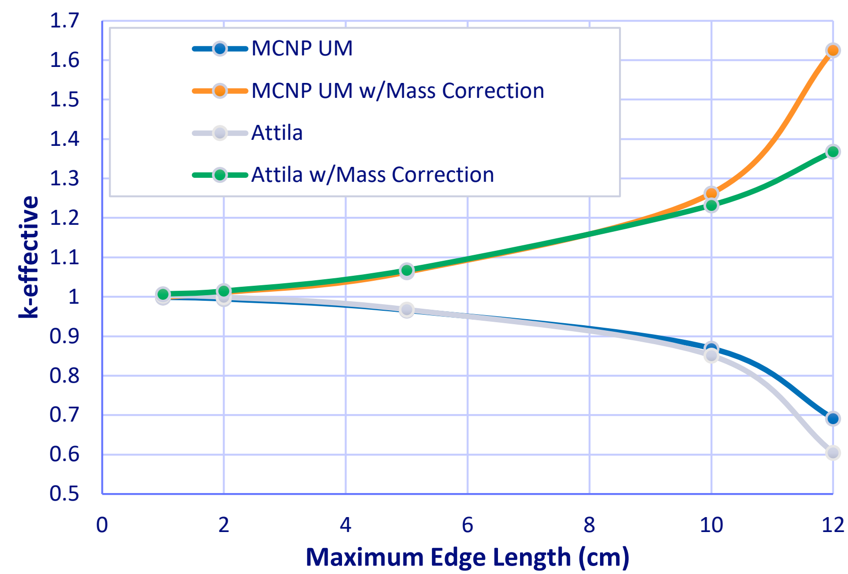
SA/Vol = 0.430



Meshed Sphere (Max Edge Length ≥ 12 cm)
Volume = 890.5 cm^3 | Area = 529.2 cm^2
SA/Vol = 0.594





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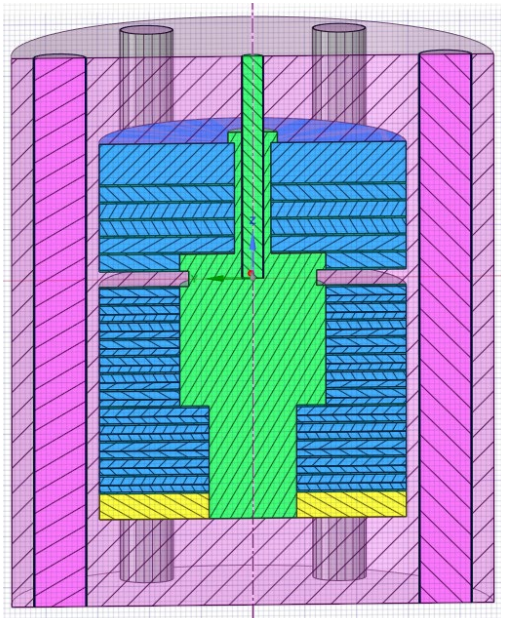
HEU-MET-FAST-007 Big Ten

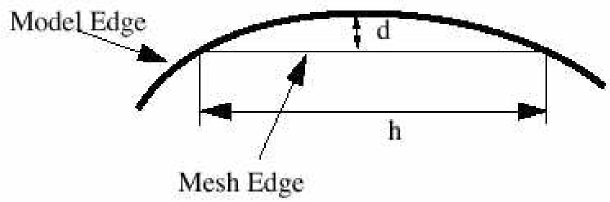
Mesh Technique: Curvature Refinement

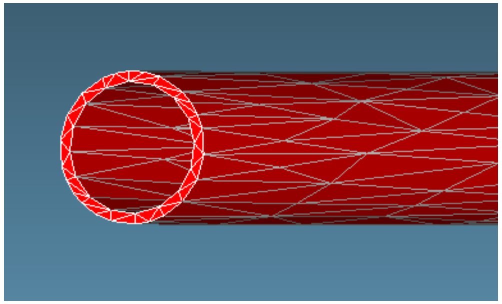
- Allows the mesh to be automatically refined to match the curvature of the entities in the geometric model. Mesh size is selected such that the distance of the model edge curve from the mesh edge (d) over the mesh edge length (h),

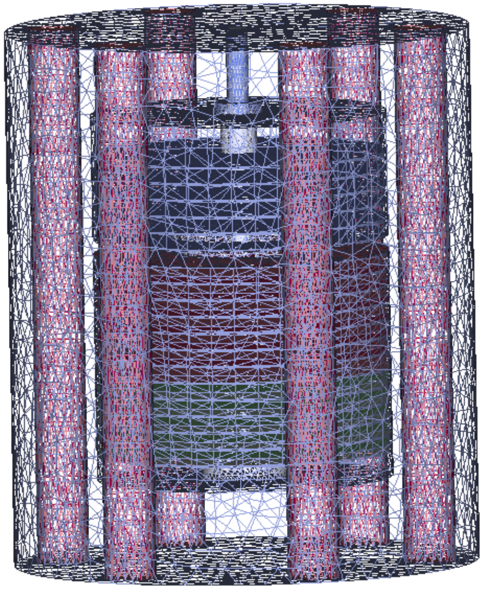
  $d/h < 0.5$

  Useful values for d/h are typically in the range of 0.01 to 0.4 (smaller value=more refinement)





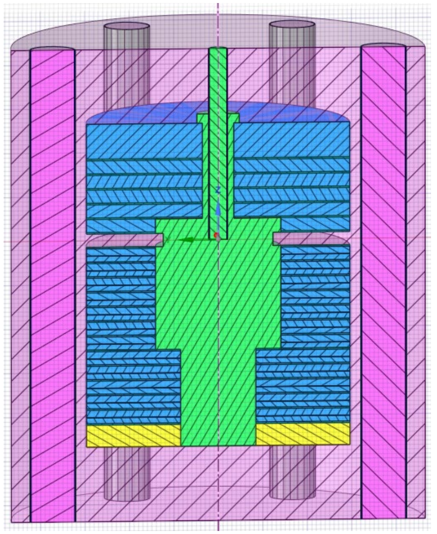


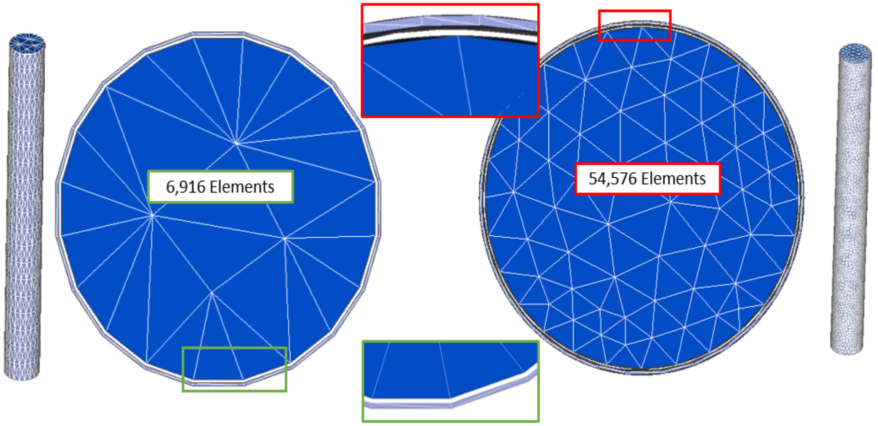


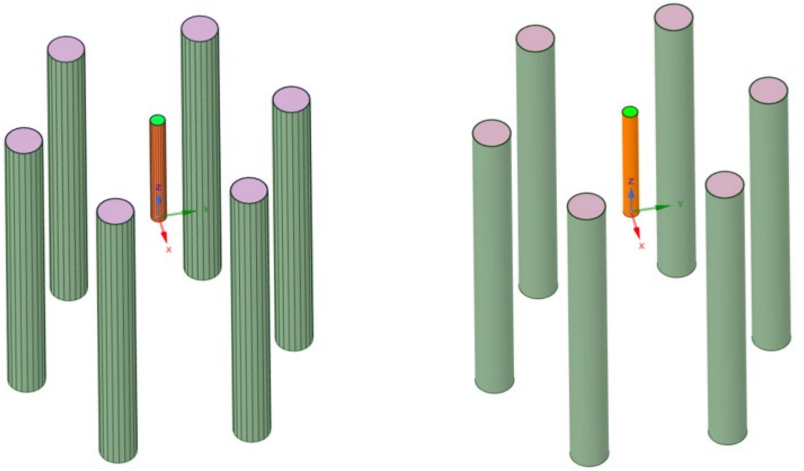
HEU-MET-FAST-007 Big Ten

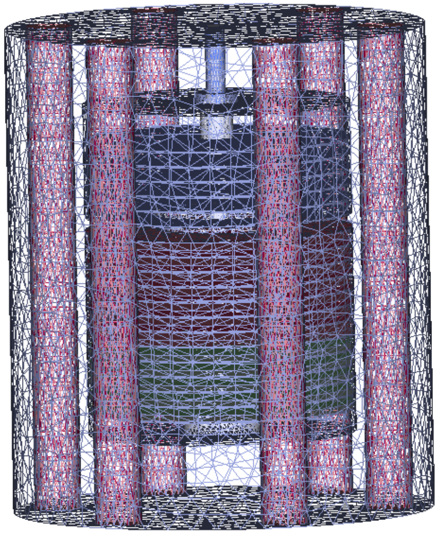
Mesh Technique: Pre-faceting

- 20-sided polygon vs. true cylinder
- Radial tolerances strictly preserved
- Mesh size substantially reduced









Critical Benchmark Results

- Critical benchmarks with various materials and geometry have been studied for use with MCNP6.2 UM
- k-effective results that are ≈ ½% experimental values **when due care is applied to mesh quality**, in preserving both the mass and shape.
- Mesh within mass and/or volume tolerances →1-2%
  - Volume within 2%, SA/V within 1%

Benchmark	CSG % k_{eff} Calc. vs. Exp	UM % k_{eff} Calc. vs. Exp	Calc/Exp k_{eff} CSG	Calc/Exp k_{eff} 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

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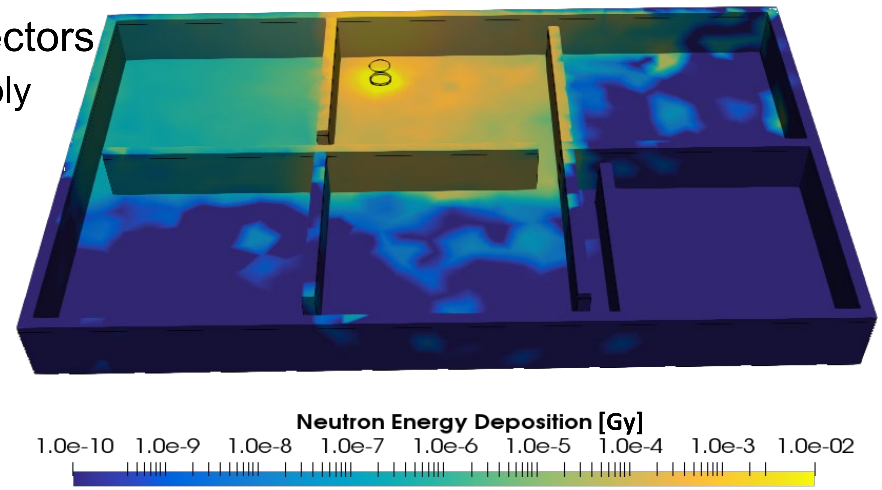
CAAS Calculations with MCNP6 Hybrid Geometry & VR

- Methods for criticality & shielding calculations
  - Criticality: excursion, source of fission neutrons/photons
  - Shielding: criticality source to detector calculations
- UM is beneficial for modeling complex facilities
  - Import existing facility CAD models
- CSG used for criticality cells, possibly detectors
  - Mass/volume preservation of critical assembly
  - Variation in detector location, mcnp_pstudy



- Steps:
1. Solid geometry
2. Mesh, MCNP input, Abaqus files
   - UM geometry embedded with CSG
3. MCNP6.2
   - KCODE calculation to create criticality source
   - Fixed source calculation for detector results using FW-CADIS weight windows
4. Visualize elemental edit out results in Paraview

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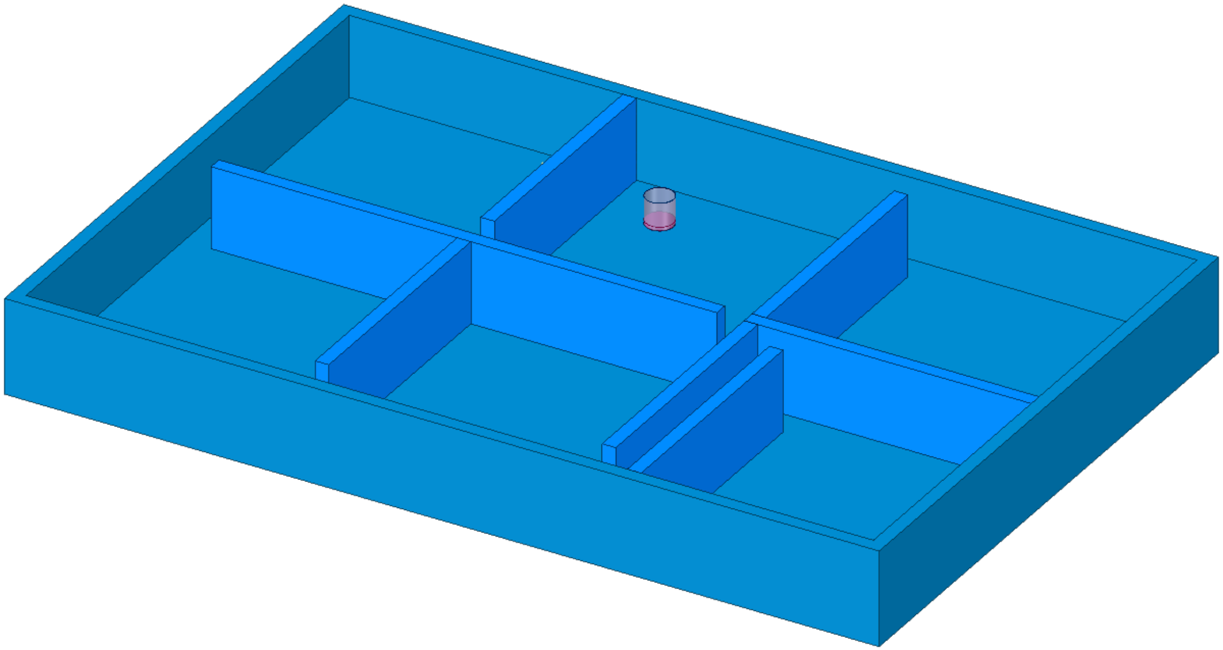
CAAS Calculations – Solid Geometry

- Model of facility
- **Unstructured Mesh**
  - 3200cm × 2150cm × 360cm
  - 10-cm thick concrete ceiling
  - 30-cm concrete walls/floor
- **CSG**
  - Pu nitrate solution
  - Stainless steel tank
  - Detector
  - Air in rooms



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CAAS Calculations – MCNP6 Hybrid Geometry

- Cell, surface, data cards:

```
c ---------------------------- Cell Cards ---------------------------------- 80
1      1      0.0764       0                                u=1
2      1      0.0764       0                                u=1
3      1      0.0764       0                                u=1
4      1      0.0764       0                                u=1
5      1      0.0764       0                                u=1
6      1      0.0764       0                                u=1
7      1      0.0764       0                                u=1
8      1      0.0764       0                                u=1
9      1      0.0764       0                                u=1
10     0                   0                                u=1 $ background
11     0                   100 -101 102 -103 104 -105   fill=1 $ fill cell
12     0                   (-100:101:-102:103:-104:105)
c -------------------------- End Cell Cards -------------------------------- 80

c --------------------------- Surface Cards -------------------------------- 80
c
100 px -1300.5
101 px 1900.5
102 py -1900.5
103 py 250.5
104 pz -50.5
105 pz 310.5
c ------------------------- End Surface Cards ------------------------------ 80

c ---------------------------- Data Cards ---------------------------------- 80
c Embedded Geometry Specification
embed1 meshgeo=abaqus mgeoin=caas_hybrid.abaq
       meeout=caas_hybrid2.mcnp.eeout
       filetype=ascii
       background=10
       matcell= 1 1 2 2 3 3 4 4 5 5 6 6 7 7 8 8 9 9
```

UM

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CAAS Calculations – MCNP6 Hybrid Geometry

… plus CSG cell & surface cards:

```
c ### cells
100      1  9.9270e-2     -10 -12                imp:n=1 $ Pu nitrate
101      3  4.8333e-5     -10 +12                imp:n=1 $ Air in tank
102      2  8.6360e-2     +10 -11                imp:n=1 $ Steel tank
120      5  -0.92         -40                    imp:n=1 $ Detector
c ### surfaces
10     rcc     0   0   2      0   0   100      50  $ inside tank
11     rcc     0   0   1      0   0   101    50.5  $ outside tank
12     pz      14.6                                $ height of solution
40     sph     -255   -300   295     5.0           $ detector
```

CSG

CAAS Calculations – MCNP6 Hybrid Geometry

```
c ----------------------------- Cell Cards ----------------------------------
1      4      0.0764          0                              u=1  imp:n=1
2      4      0.0764          0                              u=1  imp:n=1
3      4      0.0764          0                              u=1  imp:n=1
4      4      0.0764          0                              u=1  imp:n=1
5      4      0.0764          0                              u=1  imp:n=1
6      4      0.0764          0                              u=1  imp:n=1
7      4      0.0764          0                              u=1  imp:n=1
8      4      0.0764          0                              u=1  imp:n=1
9      4      0.0764          0                              u=1  imp:n=1
10     3      4.8333e-5       0                              u=1  imp:n=1 $ background
11     3      4.8333e-5       -200 11 40                 fill=1   imp:n=1 $ fill cell
100    1      9.9270e-2      -10 -12                              imp:n=1 $ Pu nitrate
101    3      4.8333e-5      -10 +12                              imp:n=1 $ air in tank
102    2      8.6360e-2      +10 -11                              imp:n=1 $ steel tank
120    5      -0.92          -40                                  imp:n=1 $ detector
200    0                     200                                  imp:n=0
c --------------------------- End Cell Cards --------------------------------

c ---------------------------- Surface Cards --------------------------------
c
10     rcc     0   0   2    0   0   100       50       $ inside tank
11     rcc     0   0   1      0   0   101     50.5     $ outside tank
12     pz      14.6                                    $ height of solution
40     sph -255   -300   295      5.0                  $ detector
200    rpp -1300.5 1900.5 -1900.5 250.5 -50.5 310.5          $ bounding box for um fill
c -------------------------- End Surface Cards ------------------------------

c ----------------------------- Data Cards ----------------------------------
c Embedded Geometry Specification
embed1 meshgeo=abaqus mgeoin=caas_hybrid.abaq
       meeout=caas_hybrid_kcode.mcnp.eeout
       filetype=ascii
       background=10
       matcell= 1 1 2 2 3 3 4 4 5 5 6 6 7 7 8 8 9 9
```

UM

CSG

CAAS Calculations – MCNP6 Calculations

MCNP6.2 KCODE calculation to obtain criticality source

- Collect fission neutrons (photons) from nitrate solution for active cycles

MCNP6.2 Fixed source calculation to obtain detector results

- Fission treatment off with ‘nonu’ card
- The energy deposited in a cell with F6 tally.
  - Neutrons from excursion: n/fission*fissions/excursion tally multiplier
- FMESH tally may be used to obtain energy deposition and relative error
  - Solution & tank w/tally multiplier & reaction numbers for energy deposition

```
fc6 neutron detector tally
f6:n 120
fm6 464638 $2.9e15 neutrons/excursion*1.6022e-10 Mev/g to Gray
fmesh104:n geom=rzt origin=0 0 1
           imesh=50 50.5 iints=10 1
           jmesh=1 13.6 100 jints=1 5 10
           kmesh=1 kints=1
           emesh 1e36 eints 1
           axs=0 0 1 vec=0 1 0
fm104 464638 0 -1 -4
```

- EEOUT file in UM to obtain energy deposition, relative error over entire

```
embee6:n embed=1 energy=464638 errors=yes
```

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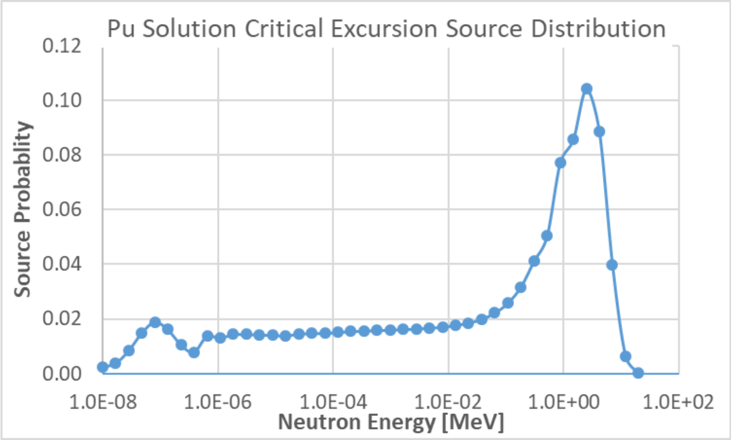
CAAS Calculations – Attila4MC FW-CADIS Calculation

- Deterministic calculation to obtain weight windows for use with MCNP6
  - Requires source spectrum obtained from earlier MCNP6 run



  - Forward weighted-Consistent Adjoint Driven Importance Sampling
    - Bias particles to obtain global solution or toward single region
    - Equal statistics throughout region
    - Requires mesh representation of entire geometry with critical cell, room air, detectors

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CAAS Calculations – MCNP6 Hybrid Geometry

- MCNP6 results w/o weight windows:

```
       6   missed  7 of 10 tfc bin checks: the relative error exceeds the recommended value of 0.1 for nonpoint detector tallies
        missed all bin error check:     1 tally bins had     0 bins with zeros and     1 bins with relative errors exceeding 0.10


 the 10 statistical checks are only for the tally fluctuation chart bin and do not apply to other tally bins.

 warning.       1 of the     1 tally fluctuation chart bins did not pass all 10 statistical checks.
 warning.       1 of the     1 tallies had bins with relative errors greater than recommended.
1tally fluctuation charts

                           tally        6
         nps      mean     error   vov  slope    fom
      1000000   1.7957E-09 0.8936 0.9734  0.0 3.2E-01
```

- MCNP6 results w/weight windows:

```
       6   passed the 10 statistical checks for the tally fluctuation chart bin result
        passed all bin error check:     1 tally bins all have relative errors less than 0.10 with no zero bins


 the 10 statistical checks are only for the tally fluctuation chart bin and do not apply to other tally bins.

1tally fluctuation charts

                           tally        6
         nps      mean     error   vov  slope    fom
      1000000   4.8070E-05 0.0962 0.0652  4.0      45
```

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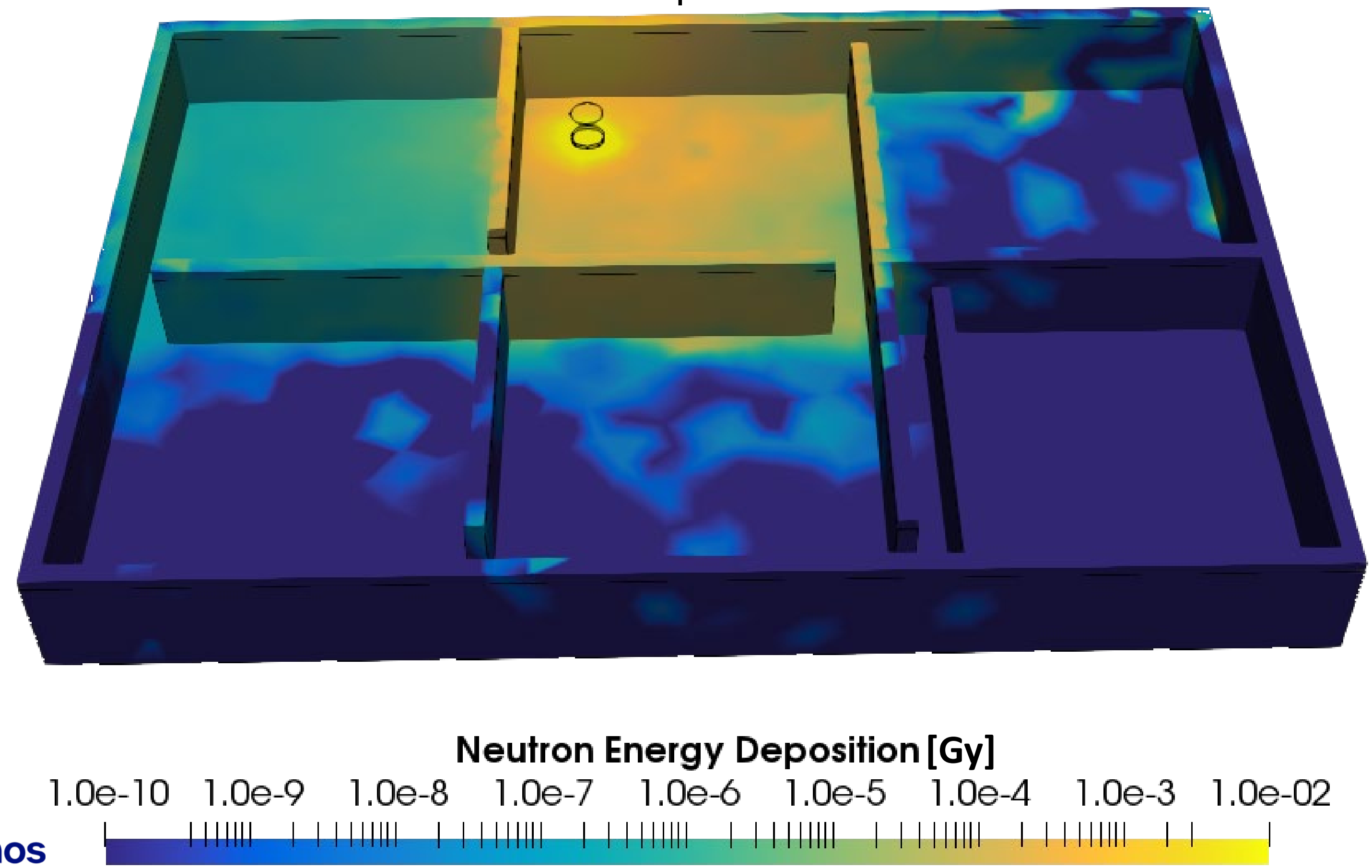
CAAS Calculations – MCNP6 Results

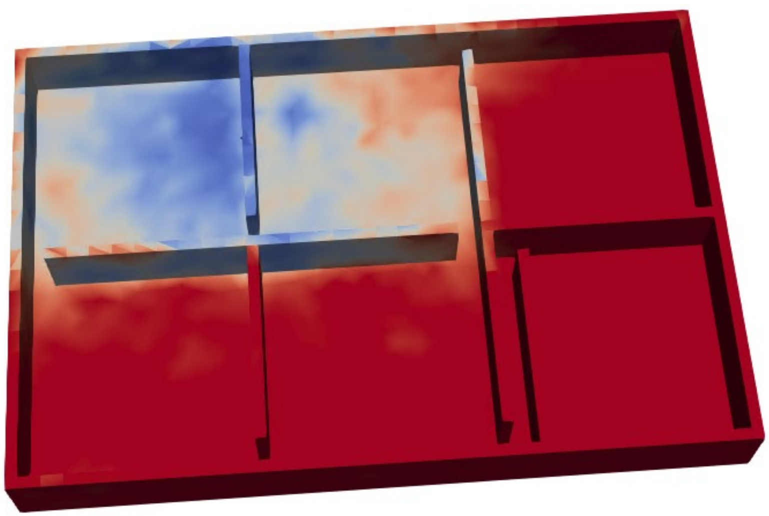
- Converted caas_hybrid.mcnp.eeout to caas_hybrid.vtu **[upcoming talk Wednesday Segment #1 Kulesza - UM Visualization and Postprocessing]**
- Visualized with Paraview
- Neutron dose results for fine mesh at 1e6 particles:



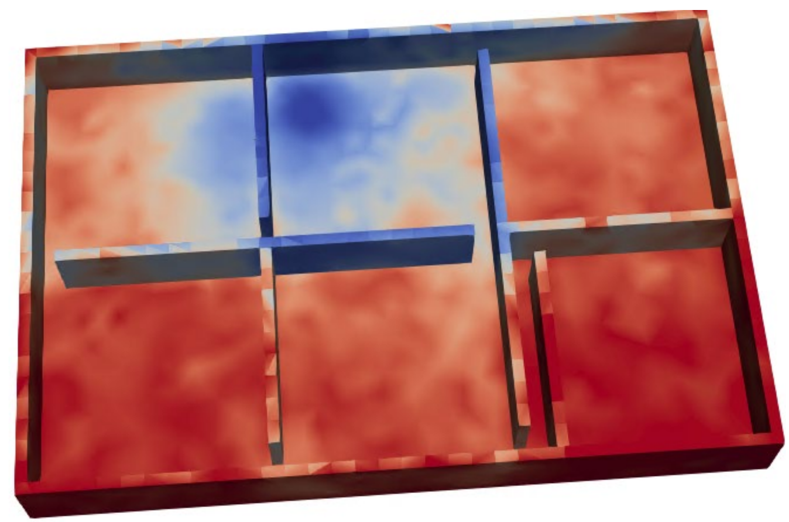
CAAS Calculations – MCNP6 Results

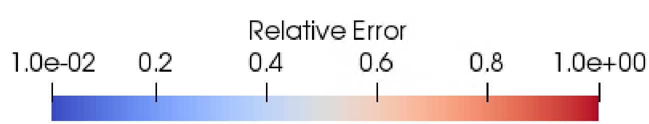
- Relative Error after 5,000,000 particles

- **FW-CADIS**:
- Custom Reports: Spatial & Energy Sets:
  - Detector
- [could use CADIS for just 1 detector]



- **FW-CADIS**:
- Custom Reports: Spatial & Energy Sets:
  - Detector + Room Air
- [best for uniform statistics throughout]





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Questions?

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