

## LA-UR-17-23854

Approved for public release; distribution is unlimited.

Title: Evaluation of the Pool Critical Assembly Benchmark with Explicitly Modeled Geometry using MCNP6's Unstructured Mesh Capabilities

Author(s): Kulesza, Joel A.  
Martz, Roger Lee

Intended for: 16th International Symposium on Reactor Dosimetry (ISR16),  
2017-05-07/2017-05-12 (Santa Fe, New Mexico, United States)

Issued: 2017-05-11 (Draft)

---

**Disclaimer:**

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

# Evaluation of the Pool Critical Assembly Benchmark with Explicitly Modeled Geometry using MCNP6's Unstructured Mesh Capabilities

Joel A. Kulesza<sup>1,2</sup> and Roger L. Martz<sup>2</sup>

<sup>1</sup>University of Michigan, Department of Nuclear Engineering & Radiological Sciences  
2355 Bonisteel Blvd., Ann Arbor, MI, 48109

<sup>2</sup>Los Alamos National Laboratory, Monte Carlo Methods, Codes, and Applications Group  
P.O. Box 1663, Los Alamos, NM, 87545

[jkulesza@umich.edu](mailto:jkulesza@umich.edu), [martz@lanl.gov](mailto:martz@lanl.gov)

16<sup>th</sup> International Symposium on Reactor Dosimetry  
May 7–12, 2017

# Outline

---

Introduction & Background

Experimental and Analytical Model

Calculational Process

Results & Summary

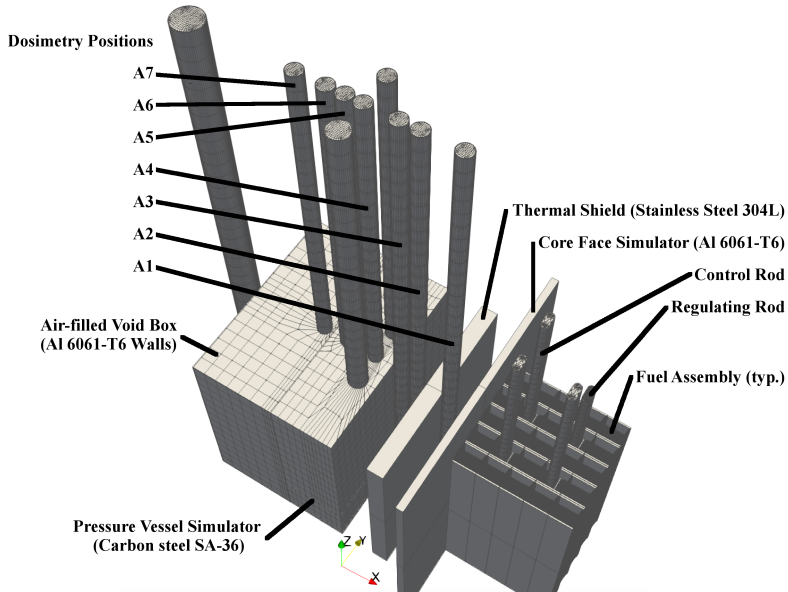
# Introduction & Background

---

**Objective: introduce reactor dosimetry community to MCNP6's unstructured mesh (UM) capabilities with a familiar benchmark problem**

- ▶ Oak Ridge National Laboratory Pool Critical Assembly
  - ▶ Originally published in 1997 by Remic and Kam (1997)
  - ▶ Recently analyzed in MCNP (using CSG) by Kulesza and Martz (2017)
- ▶ First time analyzing PCA with Monte Carlo on UM
  - ▶ It is hoped that this work will stimulate interest among the reactor dosimetry community for incorporating UM into their own analyses
- ▶ This work expands the set of MCNP6 UM validation analyses

# Geometry Overview

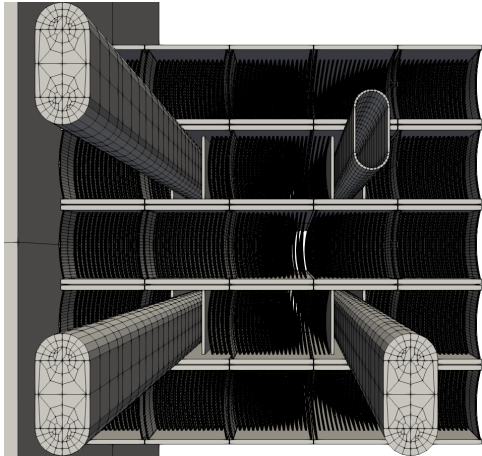


# Unstructured Mesh Modeling Process

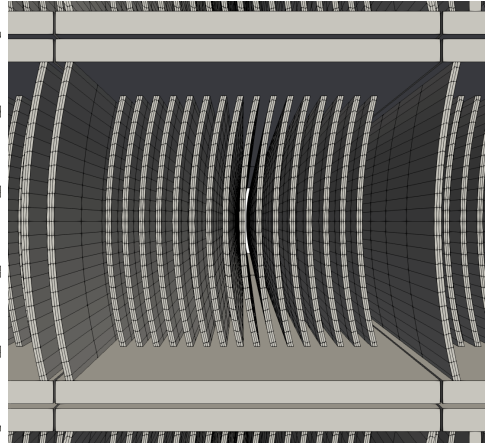
---

- ▶ UM considerations
  1. Accurate representation of geometry
  2. Sufficient granularity for results visualization
  3. Well-behaved elements
- ▶ Mesh creation process summary
  1. Create model geometry in SpaceClaim
  2. Export SpaceClaim model to STEP format
  3. Import STEP into Abaqus
  4. Define element sets and materials within Abaqus
  5. Define mesh seed spacing for each part in Abaqus
  6. Create mesh in Abaqus
  7. Combine meshed parts into assembly
  8. Write input for MCNP6
    - ▶ Steps 3–7 automated via Python within Abaqus
    - ▶ Some tuning necessary for Steps 5 & 6

# PCA Core Geometry



Top-down overview

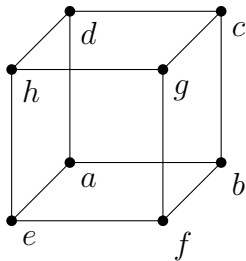


Top-down detail view of fuel assembly

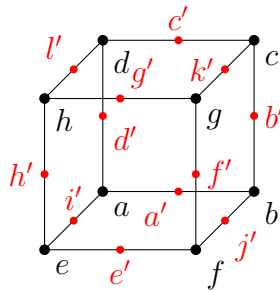


# Unstructured Mesh Statistics

- ▶ 932 SpaceClaim parts
  - ▶ Each fuel plate is two parts: fuel & cladding
  - ▶ The RPV is split into 3 parts to ease meshing: 935 total
- ▶ 745,248 first-order hexahedral elements total
  - ▶ No part with more than 12,000 elements
  - ▶ Fuel has ~450 elements
  - ▶ Fuel clad has ~1,300 elements
  - ▶ Mesh generation requires ~10 minutes



First-order hexahedron



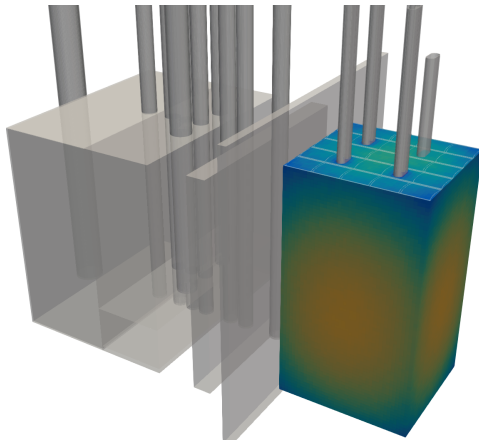
Second-order hexahedron

## Step 1: Criticality Calculation for Source Term

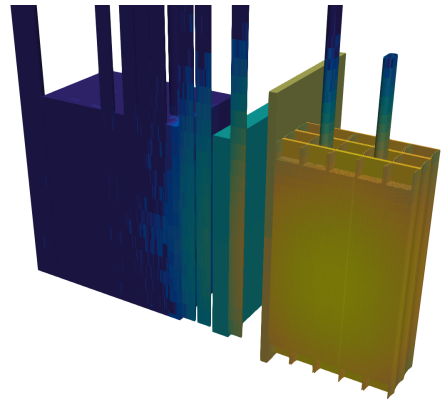
---

- ▶ Remic and Kam (1997) provide shape functions to define source
- ▶ This work calculates the fission source directly
  - ▶ Perform an eigenvalue calculation to determine source points
  - ▶ Convert source points into a fixed surface source
- ▶ Benefits of this approach
  - ▶ A near-critical eigenvalue helps validate the model
  - ▶ “Easier” to define in a Monte Carlo analysis
- ▶ Results of this approach
  - ▶ Eigenvalue usually within 50 pcm of unity
  - ▶ Eigenvalue  $1\sigma$  uncertainty of  $\sim 50$  pcm
  - ▶ Mesh tallies and UM edits can confirm source term behavior

# Visual Validation of Source Term

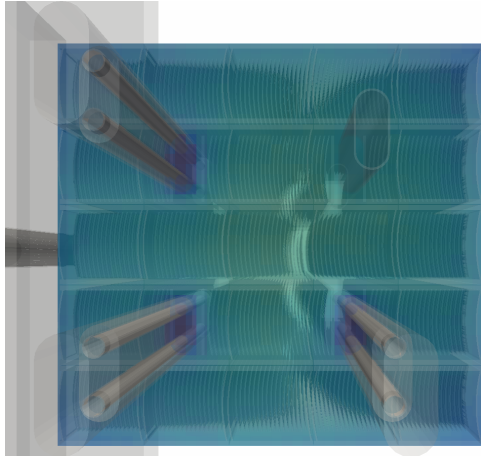


Core-wide meshtally

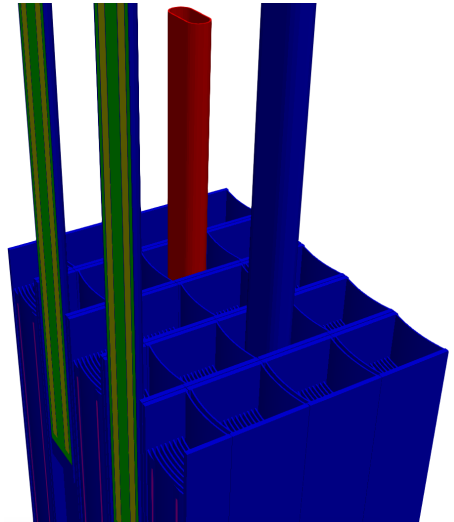


UM-wide track-length edits

# Confirmatory Views of Source Term & Geometry



Top-down view of core with transparent geometry



Geometry colored by material

## Step 2: Conversion of Fission Sites to Fixed Source

---

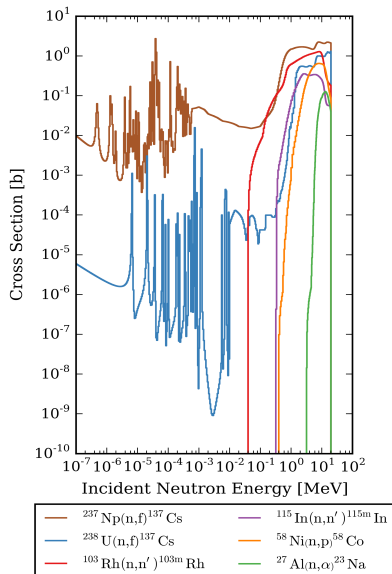
- ▶ Uses MCNP6's surface source read/write (SSR/W) capabilities
  - ▶ In this special case, SSR/W processes fission sites, not surfaces
- ▶ Process summary
  1. Set neutrons/batch and number of batches
    - ▶ Product gives number of source points processed
    - ▶ **Can lead to source particle weight adjustments**
  2. Define the cells that contain fission sites
  3. MCNP6 will read the `srctp` file and produce a surface source (`wssa`) file
- ▶ Process tutorial available in MCNP Criticality Calculations Course<sup>1</sup>
  - ▶ Problem P-16, Criticality Accident Alarm System Calculations

---

<sup>1</sup> <https://laws.lanl.gov/vhosts/mcnp.lanl.gov/classes/classinformation.shtml>

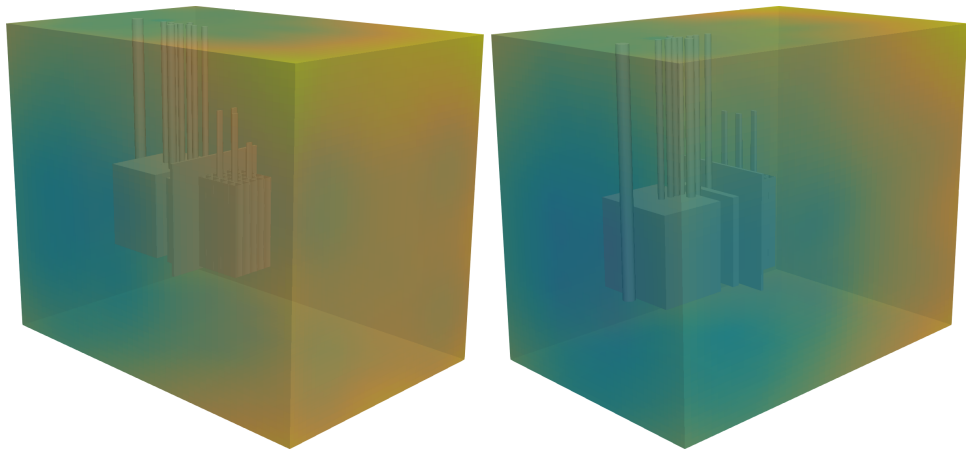
## Step 3: Final Fixed Source Calculations

- ▶ Reuse ADVANTG-produced weight windows from Kulesza and Martz (2017)
  - ▶ One set of weight windows per reactions
  - ▶ Constructed based on IRDFF v.1.05 dosimetry responses
- ▶ 180 total calculations, 512 processors each
  - ▶ 30 independent 1-million history runs  $\times$  6 reactions
  - ▶ Total computer time: 554.5 hours (283,892 core hours)



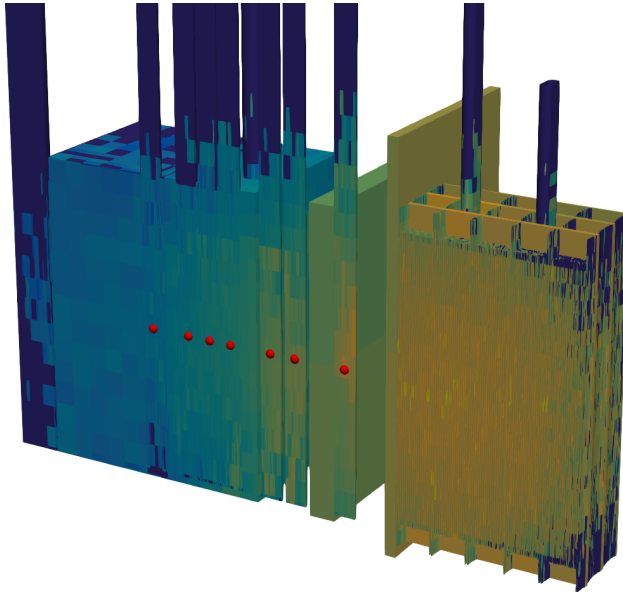
# Reasonable Weight Window Behavior

---



- ▶ Problem domain:  $-150 \leq x \leq 150$ ,  $-100 \leq y \leq 100$ ,  $-100 \leq z \leq 150$

# Unstructured Mesh Flux Edit — $^{27}\text{Al}(n,\alpha)$ Execution





## Calculation / Experiment (Remic and Kam, 1997) Ratios

Loc.	$^{27}\text{Al}(n,\alpha)$	$^{58}\text{Ni}(n,p)$	$^{103}\text{Rh}(n,n')$	$^{115}\text{In}(n,n')$	$^{238}\text{U}(n,f)$	$^{237}\text{Np}(n,f)$	Avg.
A1	0.91	1.00	1.11	1.04	—	1.08	1.03
A2	0.99	1.09	—	1.03	—	—	1.04
A3	1.04	1.11	—	1.14	—	1.27	1.14
A4	1.29	1.11	1.09	1.06	1.04	1.11	1.12
A5	1.15	1.12	1.04	1.10	0.97	1.08	1.08
A6	—	1.18	1.06	1.06	1.01	1.10	1.08
A7	—	—	—	—	—	1.30	1.30
Avg.	1.08	1.10	1.08	1.07	1.01	1.16	1.09

- ▶  $^{27}\text{Al}$  values have higher-than-desired statistical uncertainties
- ▶  $^{237}\text{Np}$  values have been observed to disagree historically
- ▶ Average agreement (by reaction, position, and overall) still reasonable

## Calculation / Experiment (Fero et al., 2001) Ratios

Loc.	$^{27}\text{Al}(n,\alpha)$	$^{58}\text{Ni}(n,p)$	$^{103}\text{Rh}(n,n')$	$^{115}\text{In}(n,n')$	$^{238}\text{U}(n,f)$	$^{237}\text{Np}(n,f)$	Avg.
A1	0.92	1.01	1.11	1.05	—	—	1.02
A2	1.00	1.09	1.15	1.04	—	—	1.07
A3	1.05	1.12	1.17	1.16	1.19	1.24	1.16
A4	1.30	1.13	1.09	1.06	1.08	1.13	1.13
A5	1.13	1.14	1.02	1.10	1.03	1.12	1.09
A6	—	1.20	1.02	1.05	1.06	1.12	1.09
A7	—	—	1.05	1.09	1.04	1.29	1.12
Avg.	1.08	1.12	1.09	1.08	1.08	1.18	1.10

- ▶  $^{27}\text{Al}$  values have higher-than-desired statistical uncertainties
- ▶  $^{237}\text{Np}$  values have been observed to disagree historically
- ▶ Average agreement (by reaction, position, and overall) still reasonable

# Summary & Future Work

---

- ▶ Demonstrated MCNP6 UM ability to perform reactor dosimetry analyses
  - ▶ Situation-specific source generation & analysis workflow
  - ▶ Techniques for validation
  - ▶ Flexibility in geometry & results visualization
- ▶ Extended MCNP6 UM validation (overall C/E ~1.10)
  - ▶ More work is needed to reduce statistical uncertainties
    - ▶ Especially true of  $^{27}\text{Al}(n,\alpha)$
    - ▶ Value in introducing track-length tallies to verify point detectors
- ▶ Short-term future work
  - ▶ Need to investigate why calculation-to-experiment ratios  $>1$
- ▶ Longer-term future work
  - ▶ More effective workflow to generate weight windows
  - ▶ Should weight windows be generated on the UM? How?

# Questions?

---

## Contact Information

Joel A. Kulesza

Mobile: +1 (734) 223-7312    Email: [jkulesza@umich.edu](mailto:jkulesza@umich.edu)

Roger L. Martz

Office: +1 (505) 664-0900    Email: [martz@lanl.gov](mailto:martz@lanl.gov)

# Backup Slides

# References

---

- Fero, A. H., Anderson, S. L., Roberts, G. K., 2001. Analysis of the ORNL PCA Benchmark Using TORT and BUGLE-96. In: Williams, J. G., Vehar, D. W., Ruddy, F. H., Gilliam, D. M. (Eds.), Reactor Dosimetry: Radiation Metrology and Assessment. American Society for Testing and Materials, West Conshohocken, PA, USA, pp. 360–366.
- Kulesza, J. A., Martz, R. L., March 2017. Evaluation of the Pool Critical Assembly Benchmark with Explicitly Modeled Geometry Using MCNP6. Nuclear Technology 197 (3), 284–295.
- Remic, I., Kam, F. B. K., July 1997. Pool Critical Assembly Pressure Vessel Facility Benchmark. Tech. Rep. NUREG/CR-6454, Oak Ridge National Laboratory, Oak Ridge, TN, USA.