List-Mode Simulations of the Subcritical Thor Core Benchmark Sensitivity Experiments

Rian M. Bahran[1], Jesson Hutchinson[2], Benoit Richard[1] & Avneet Sood[1]

Los Alamos National Laboratory

[1]X-Computational Physics Division, Monte Carlo Methods, Codes and Applications Group (XCP-3)

[2]Nuclear Engineering and Non-Proliferation Division, Advanced Nuclear Technology Group (NEN-2)

Presented at the American Nuclear Society Winter Meeting in Anaheim, CA

November 11th, 2014

LA-UR-14-28651

General Overview

- **Sub-critical multiplying systems provide valuable information.**
  - Validation of nuclear data and codes.
  - Uncertainty quantification for various applications.
  - Design of future measurements.

- **Monte Carlo simulations of an experimental subcritical benchmark were performed.**
  - Helps validate recent improvements in computational tools.
  - Provides better predictability and understanding in the sensitivities and uncertainties associated with subcritical systems.

- **Experiments/simulations involved extensive mass and geometry perturbations.**
  - 40+ different configurations: detailed model of the system & associated perturbations.
  - MCNP5 with list-mode patch used for simulations.

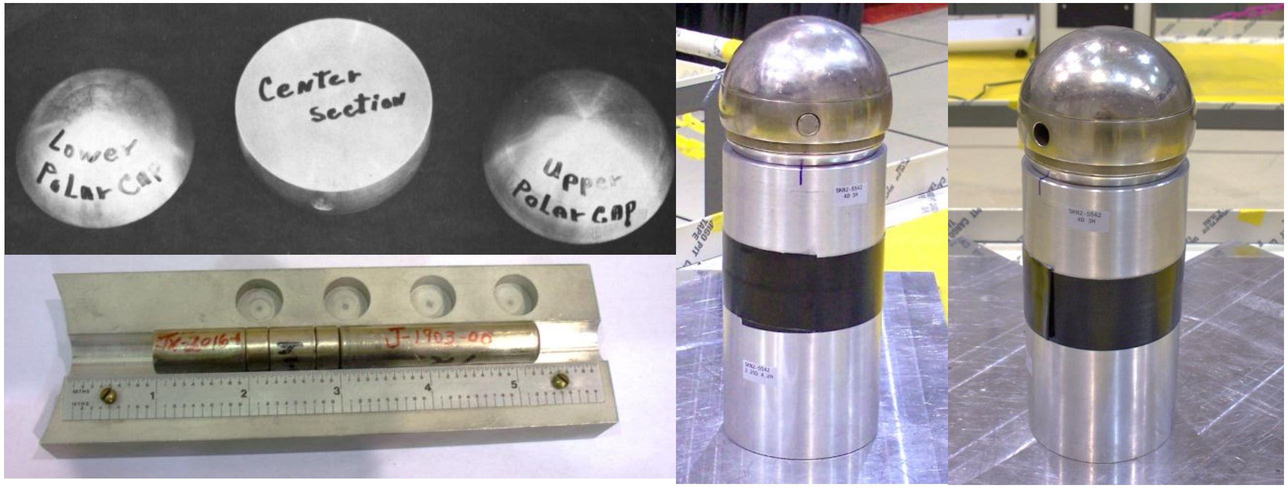
- **^{3}He neutron multiplicity detectors provided list-mode data in exp. & simulation.**
  - Time stamp (and location) of every registered event.

- **Data analyzed using the Feynman Variance-to-Mean method to obtain M_T.**

Subcritical System in Nevada: Thor Pu-metal core

- **TA-18 operated at LANL from 1945-2005**
  - 2004-2005: Shipment of nuclear material from TA-18 to DAF.
  - 2011: Critical experiment capability resumed at DAF.

- **Assembled Thor pieces approximate a sphere ~10.6 cm in diameter.**
  - Total net mass (with inserts) 9649.0 g.



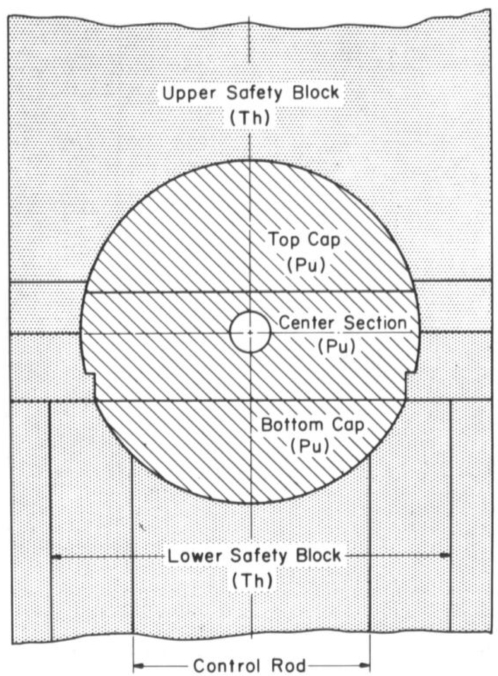
- **Isotopic composition similar to Jezebel/BeRP.**
  - 5.1% ^{240}Pu (alloyed with ~1.01 wt% gallium), components clad with ~5 mils of Ni.

Several major Thor Core experiment and evaluation publications are available in the literature.

NUCLEAR SCIENCE AND ENGINEERING: **71**, 287-293 (1979)

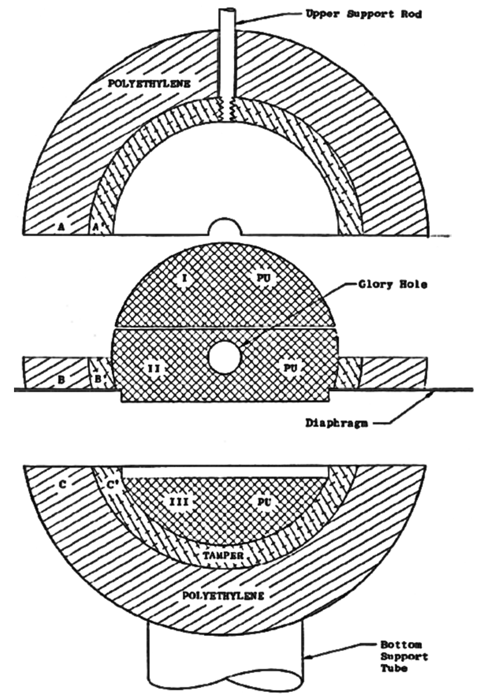
Thor, A Thorium-Reflected Plutonium-Metal Critical Assembly

G. E. Hansen and H. C. Paxton
University of California, Los Alamos Scientific Laboratory, P.O. Box 1663 Los Alamos, New Mexico 87545



PU-MET-FAST-008

Benchmark Critical Experiment of a Thorium Reflected Pu Sphere



PU-MET-FAST-044

Pu Metal Sphere with Be, Graphite, Al, Fe and Mo Tampers and Polyethylene Reflectors

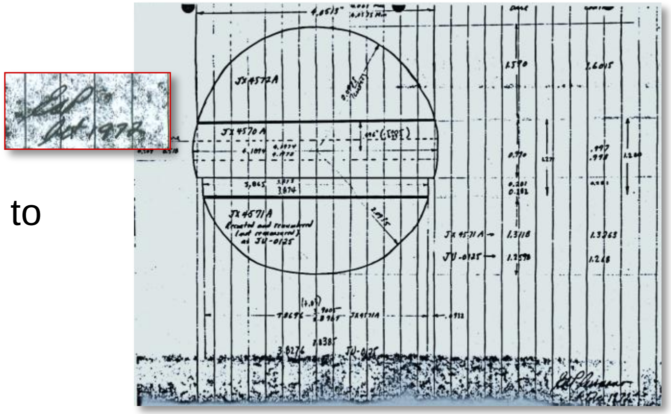
UNCLASSIFIED

Los Alamos NATIONAL LABORATORY EST.1943

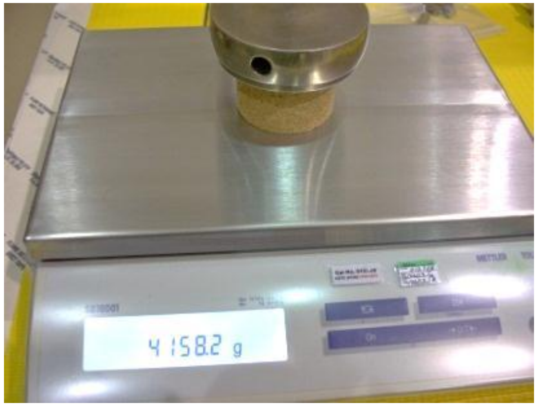
Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

A geometry revaluation of the Thor core major components geometry was performed.

- **Updated dimensions determined from:**
  - Original unpublished drawings from 1972.
  - Unpublished documents from 2005 when material was transferred from Los Alamos to the Nevada National Security Site.

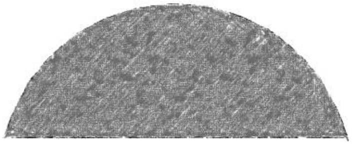


- **Updated mass and density values also obtained for the Thor components from:**
  - Mass measurements.
  - Stochastic volume ray-tracing estimation method with MCNP.
  - Analytical calculations.

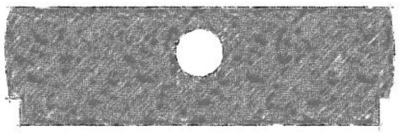


Updated Thor mass and volume from a recent geometry re-evaluation.

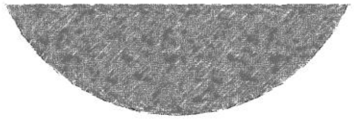
Upper Spherical Cap (JX-4572)				
Volume	**Coated [cm³]**	**Ni [cm³]**	**Pu-alloy [cm³]**	
present work: MCNP5	206.4 ± 0.1	2.67 ± 0.01	203.7 ± 0.12	
Mass	**Coated [g]**	**Ni [g]**	**Pu-alloy [g]**	**Pu [g]**
present work: measurement / MCNP5	3273.9 ± 0.1	23.78 ± 0.1	3249.2 ± 0.14	3216
unpublished work (2005)	3274.0	25.25	3249	3216.2
unpublished work (1972)			3225	3192.4
Robba et al. (1983)			3225	3193



Center Component (JX-4570)				
Volume	**Coated [cm³]**	**Ni [cm³]**	**Pu-alloy [cm³]**	
present work: MCNP5	262.4 ± 0.13	3.58 ± 0.01	258.8 ± 0.13	
Mass	**Coated [g]**	**Ni [g]**	**Pu-alloy [g]**	**Pu [g]**
present work: measurement / MCNP5	4158.2 ± 0.1	31.9 ± 0.1	4126.3 ± 0.14	4085
unpublished work (2005)	4158.3	33.71	4124.6	4083
unpublished work (1972)			4127	4085.3
Robba et al. (1983)			4127	4086



Lower Spherical Cap (JU-125)				
Volume	**Coated [cm³]**	**Ni [cm³]**	**Pu-alloy [cm³]**	
present work: MCNP5	137.9 ± 0.1	2.22 ± 0.01	135.7 ± 0.1	
Mass	**Coated [g]**	**Ni [g]**	**Pu-alloy [g]**	**Pu [g]**
present work: measurement / MCNP5	2216.9 ± 0.1	19.7 ± 0.1	2197.2 ± 0.14	2175
unpublished work (2005)	2216.9	20.44	2196.5	2174.3
unpublished work (1972)	2216.75	20.85	2195.9	2173.7
Robba et al. (1983)			2196	2174



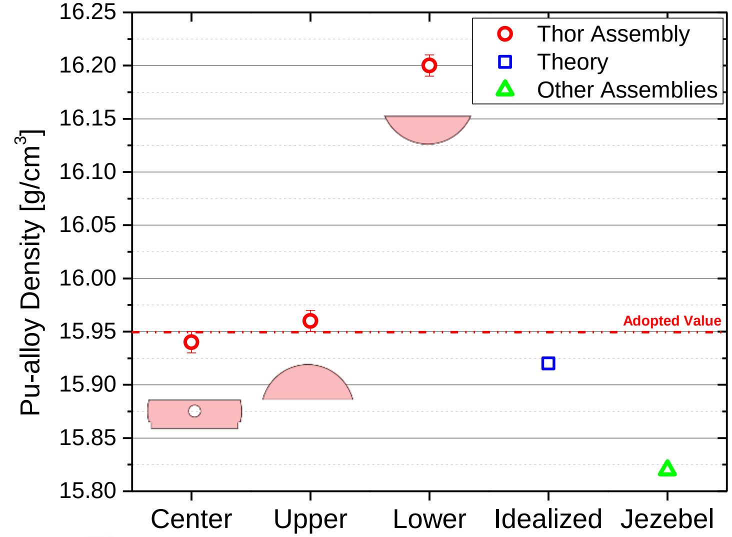
An updated Thor density of 15.95 g/cm³ was obtained.

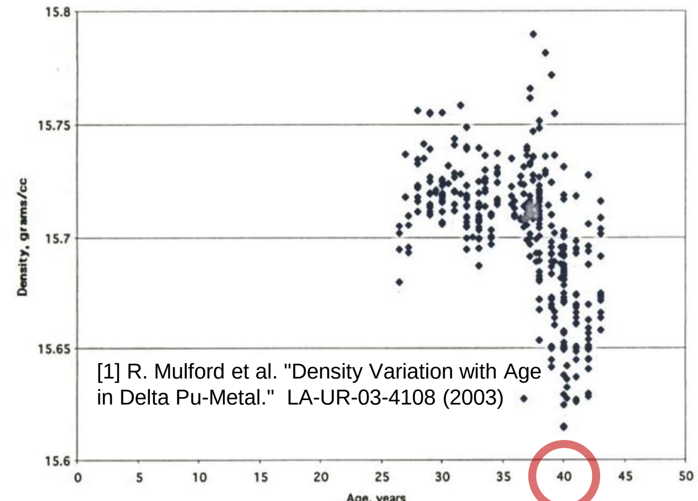
- **Calculated $\rho_{Pu\text{-}alloy}$ for Center/Upper components within statistical uncertainties.**
  - Mass-averaged value of 15.95 g/cm³.

- **Discrepancy in Lower piece.**
  - Likely attributed to dimension inaccuracies.
  - Component was stripped of its original Ni cladding leading to material loss.

- **Density of δ-phase plutonium metal decreases as a function of time due to void swelling from helium buildup [1].**
  - Average rate of density loss after 35 years ~0.01 g/cm³ per year.
  - Can vary locally for a specific sample.
  - MISC [2] was used to decay initial Pu isotopes of the 40+ year old Thor core.

[2] C. Solomon “MCNP Intrinsic Source Constructor (MISC):A User's Guide” LA-UR-12-20252 (2012)

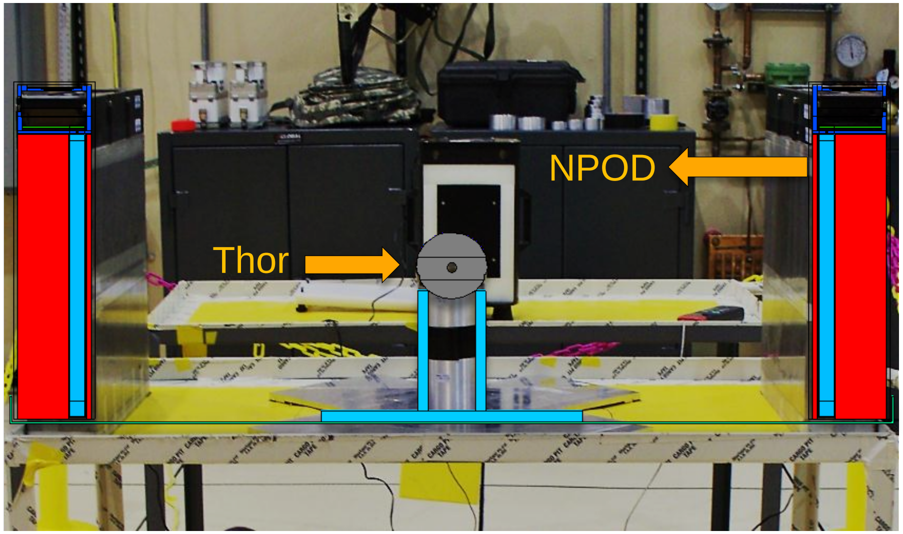




[1] R. Mulford et al. "Density Variation with Age in Delta Pu-Metal." LA-UR-03-4108 (2003)

Configuration of Thor Pu-metal core measurements.

- **14 main configurations were measured (various combinations of Thor core pieces).**
- **40+ perturbation configurations:**
  - Varying mass (different glory hole loadings).
  - Varying geometry (S-to-D distance).
  - Measurements with only 1 NPOD.
- **4 Detectors used:**
  - 2 x NPOD (LANL neutron multiplicity detector).
  - 1 x SNAP (LANL gross neutron counter).
  - 1 x HPGe (ORTEC gamma detector).
- **List-mode data obtained from NPOD measurements and simulations with MCNP**
  - Hage-Cifarelli formalism of the Feynman variance-to-mean method was used in analysis.
  - Single value for efficiency (all bare configurations).
    - Measured using a neutron source: 0.0091 +/- 0.0005
    - Validated using a combination of the SNAP/NPOD count rates for each configuration.



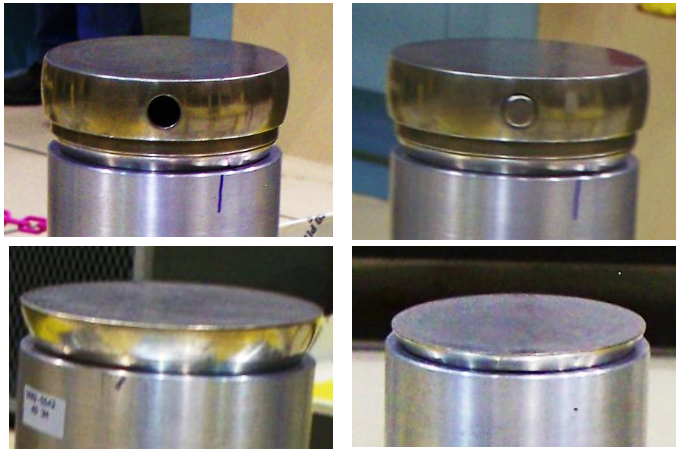
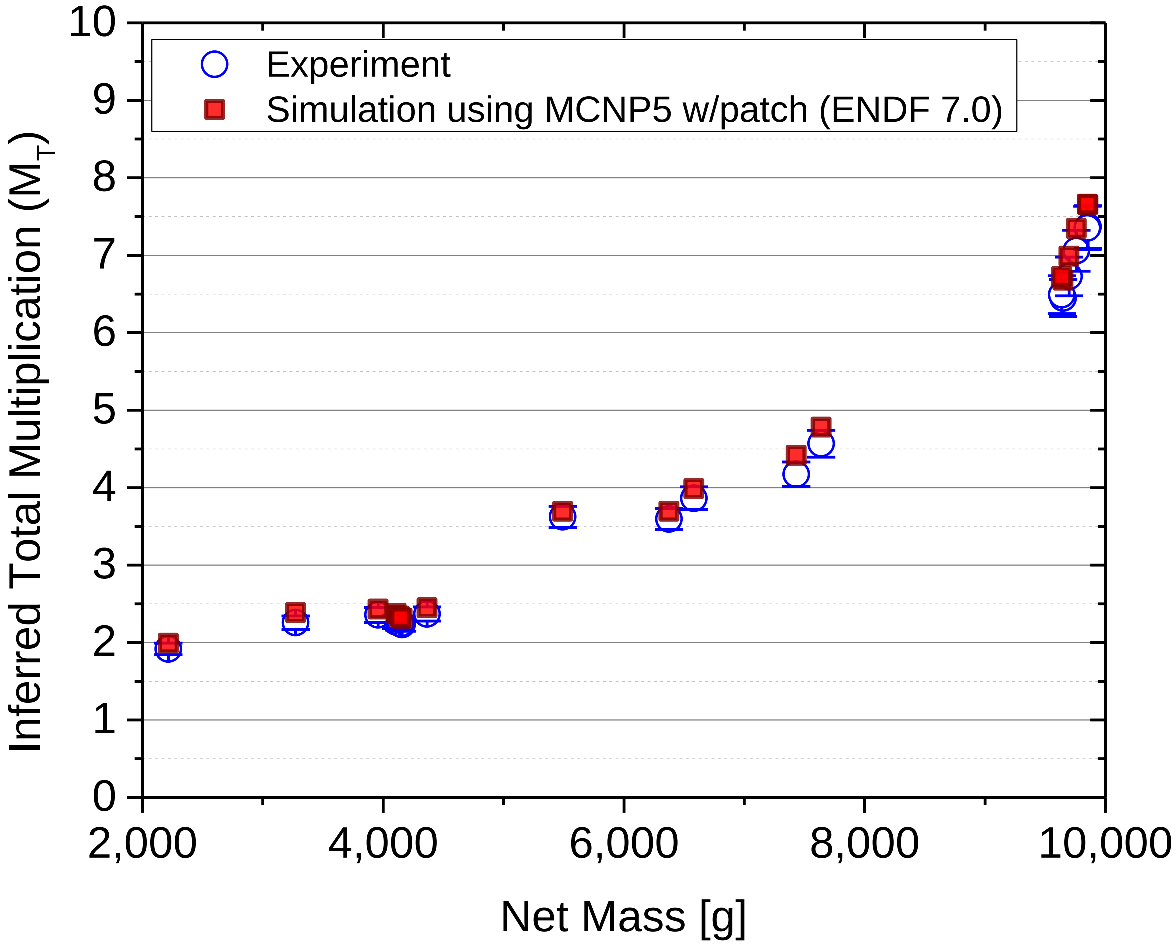


Table of the different configuration perturbations.

		Thor Core				Glory Hole			NPOD	
CONFIG. #	PERT.	Lower	Center	Upper	→	Loading	Mass [g]	Direction	S/D [cm]	#
1		+			def=vertical	None	0	def=NE-SW ↗	def=50	def=2
2			+		def=vertical	None	0	def=NE-SW ↗	def=50	def=2
3			+		def=vertical	Full	206.9	def=NE-SW ↗	def=50	def=2
	3p1		+		def=vertical	Full	206.9	N-S ↕	def=50	def=2
	3p2		+		def=vertical	Full	206.9	E-W ↔	def=50	def=2
	3p3		+		def=vertical	Full	206.9	def=NE-SW ↗	49.5	def=2
	3p4		+		def=vertical	Full	206.9	def=NE-SW ↗	49	def=2
	3p5		+		def=vertical	Full	206.9	def=NE-SW ↗	48	def=2
	3p6		+		def=vertical	Full	206.9	def=NE-SW ↗	45	def=2
	3p12		+		def=vertical	Quarter	49	def=NE-SW ↗	def=50	def=2
	3p13		+		def=vertical	Altern. Full	200.7	def=NE-SW ↗	def=50	def=2
	3p15		+		def=vertical	1/8th	24.7	def=NE-SW ↗	def=50	def=2
	3p16		+		def=vertical	1/16th	11.8	def=NE-SW ↗	def=50	def=2
	3p17		+		def=vertical	Full	206.9	E-W ↔	def=50	def=2
4				+	def=vertical	None	0	def=NE-SW ↗	def=50	def=2
5		+	+		def=vertical	None	0	def=NE-SW ↗	def=50	def=2
6		+	+		def=vertical	Full	206.9	def=NE-SW ↗	def=50	def=2
7		+		+	def=vertical	None	0	def=NE-SW ↗	def=50	def=2
	7p1	+		+	inverted ↓	None	0	def=NE-SW ↗	def=50	def=2
8			+	+	def=vertical	None	0	def=NE-SW ↗	def=50	def=2
9			+	+	def=vertical	Full	206.9	def=NE-SW ↗	def=50	def=2
10		+	+	+	def=vertical	None	0	def=NE-SW ↗	def=50	def=2
	10p1	+	+	+	def=vertical	None	0	E-W ↔	def=50	def=2
	10p2	+	+	+	def=vertical	None	0	N-S ↕	def=50	def=2
11		+	+	+	def=vertical	Full	206.9	def=NE-SW ↗	def=50	def=2
	11p2	+	+	+	def=vertical	1/16th	11.8	def=NE-SW ↗	def=50	def=2
	11p3	+	+	+	def=vertical	Alt. Full	200.7	def=NE-SW ↗	def=50	def=2
	11p4	+	+	+	def=vertical	Full	206.9	N-S ↕	def=50	def=2
	11p5	+	+	+	def=vertical	Full	206.9	E-W ↔	def=50	def=2
	11p6	+	+	+	def=vertical	Full	206.9	def=NE-SW ↗	49.5	def=2
	11p7	+	+	+	def=vertical	Full	206.9	def=NE-SW ↗	49	def=2
	11p8	+	+	+	def=vertical	Full	206.9	def=NE-SW ↗	48	def=2
	11p9	+	+	+	def=vertical	Full	206.9	def=NE-SW ↗	45	def=2
	11p14	+	+	+	inverted ↓	Full	206.9	def=NE-SW ↗	def=50	def=2
	11p15	+	+	+	def=vertical	Full	206.9	def=NE-SW ↗	def=50	1
12		+	+	+	def=vertical	Half	109.5	def=NE-SW ↗	def=50	def=2
13		+	+	+	def=vertical	Quarter	49	def=NE-SW ↗	def=50	def=2
14					def=vertical	Full	206.9	def=NE-SW ↗	def=50	def=2
	14p1				def=vertical	Full	206.9	N-S ↕	def=50	def=2
	14p2				def=vertical	Full	206.9	E-W ↔	def=50	def=2
	14p3				def=vertical	Half	109.5	def=NE-SW ↗	def=50	def=2
	14p4				def=vertical	Quarter	49	def=NE-SW ↗	def=50	def=2
	14p5				def=vertical	Altern. Full	200.7	def=NE-SW ↗	def=50	def=2

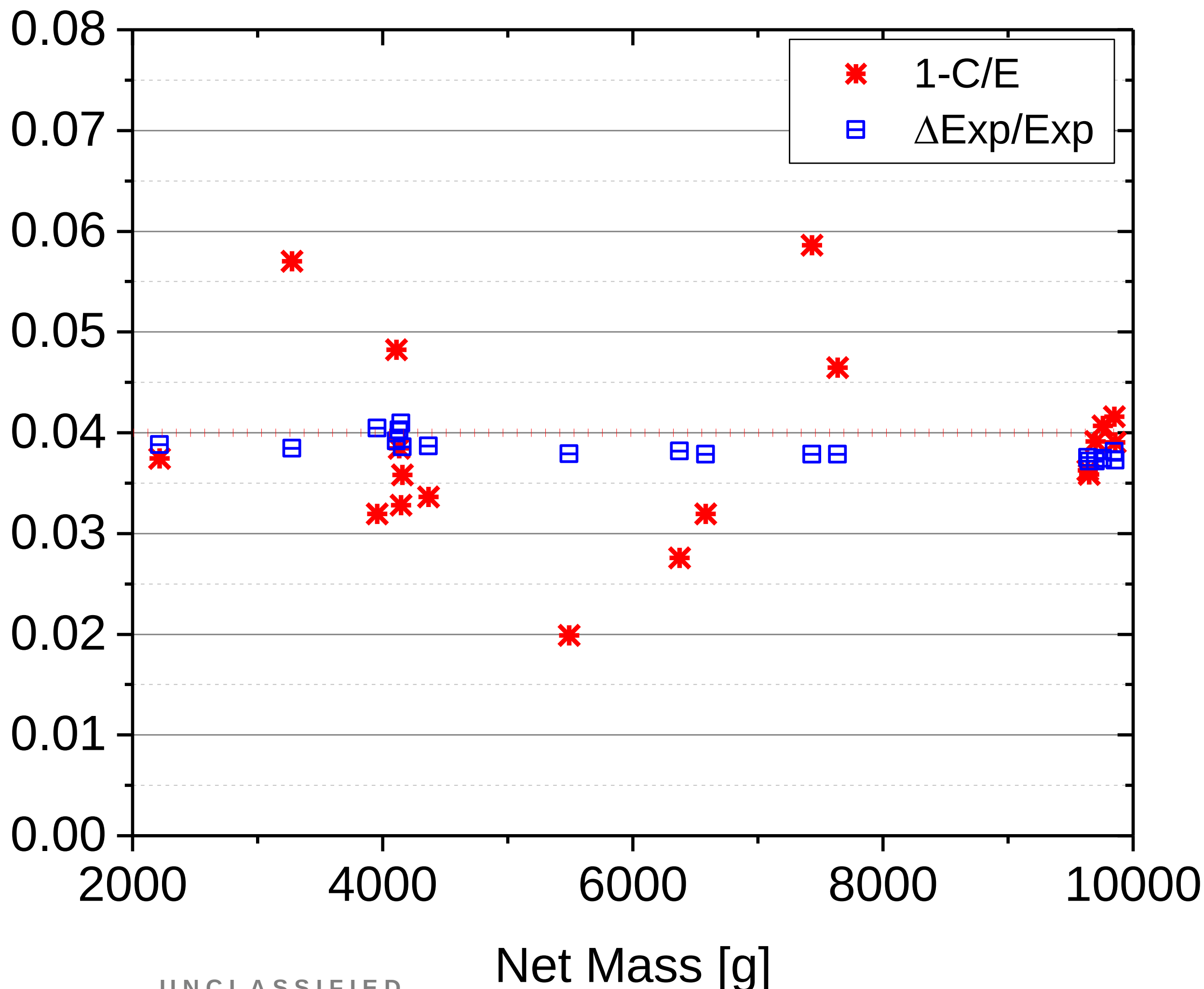
Total Neutron Multiplication (Inferred) vs System Mass



Calculation/Experiment for Total Multiplication

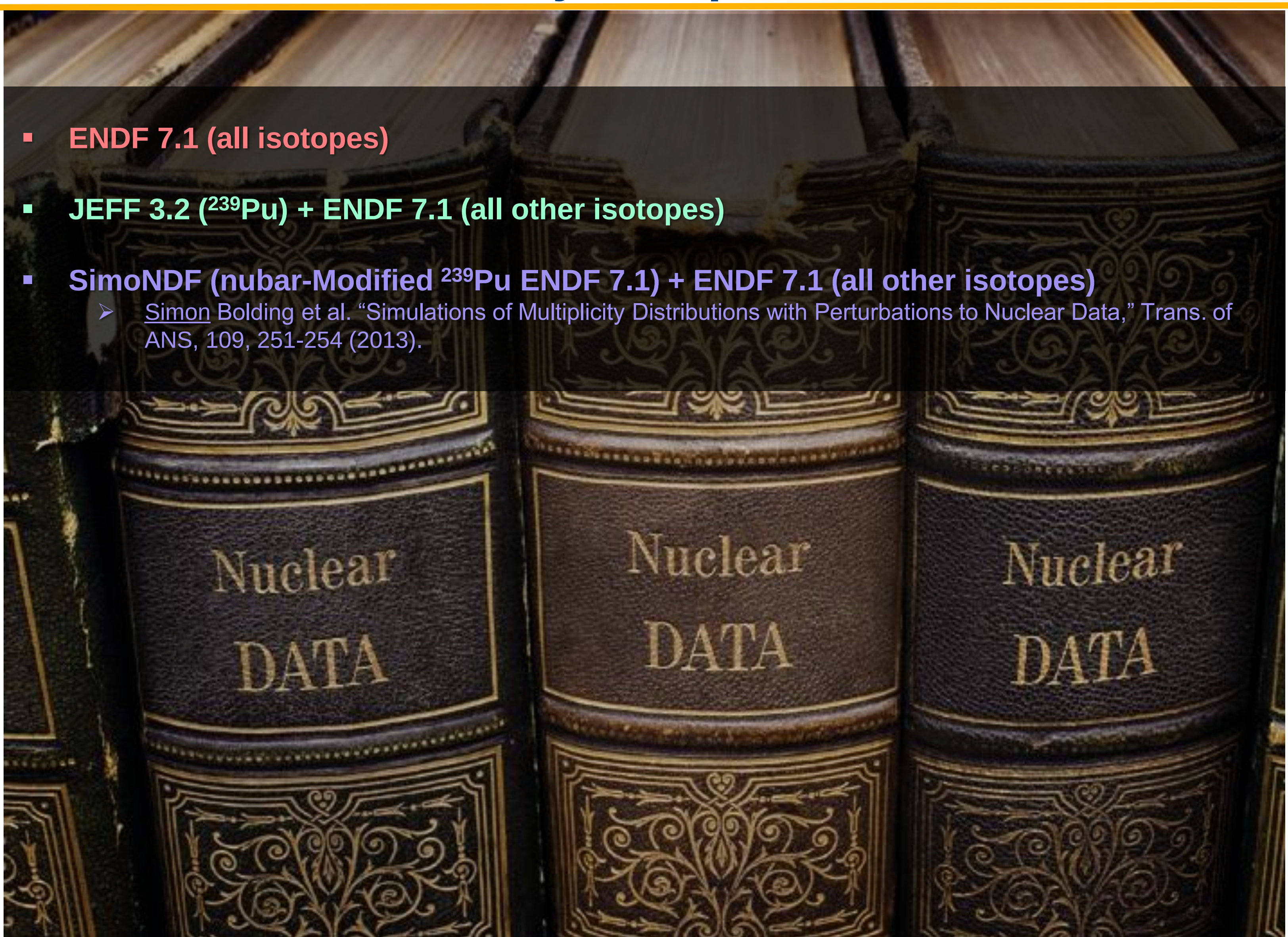
Calculation ~4% higher

- Consistent with past comparisons.
- Barely within the measurement uncertainty.

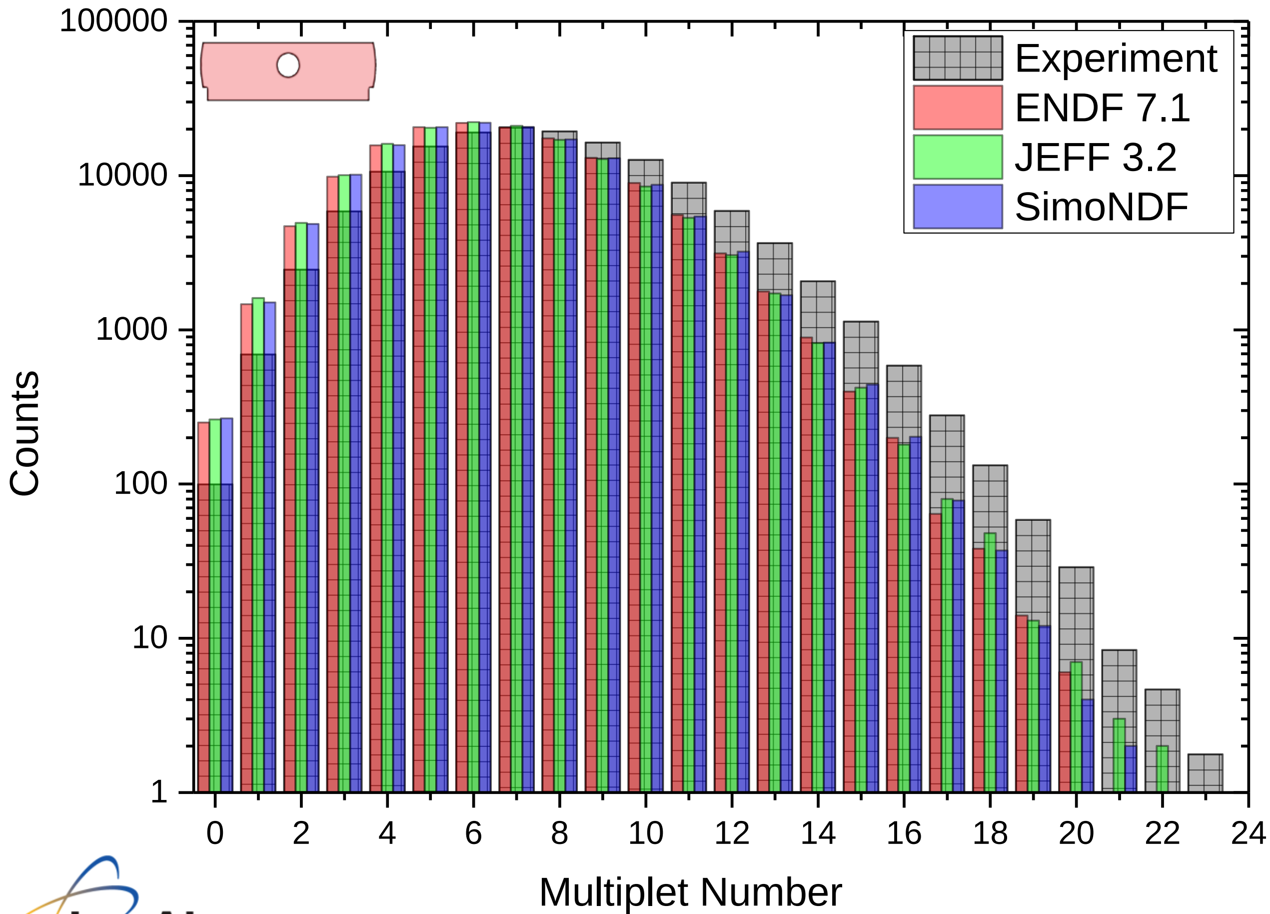


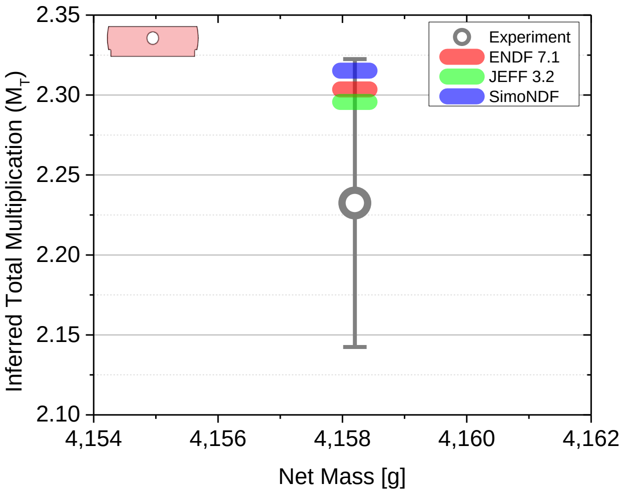
^{239}Pu Nuclear Data Library Comparisons

- ENDF 7.1 (all isotopes)
- JEFF 3.2 (^{239}Pu) + ENDF 7.1 (all other isotopes)
- SimoNDF (nubar-Modified ^{239}Pu ENDF 7.1) + ENDF 7.1 (all other isotopes)
  - Simon Bolding et al. “Simulations of Multiplicity Distributions with Perturbations to Nuclear Data,” Trans. of ANS, 109, 251-254 (2013).



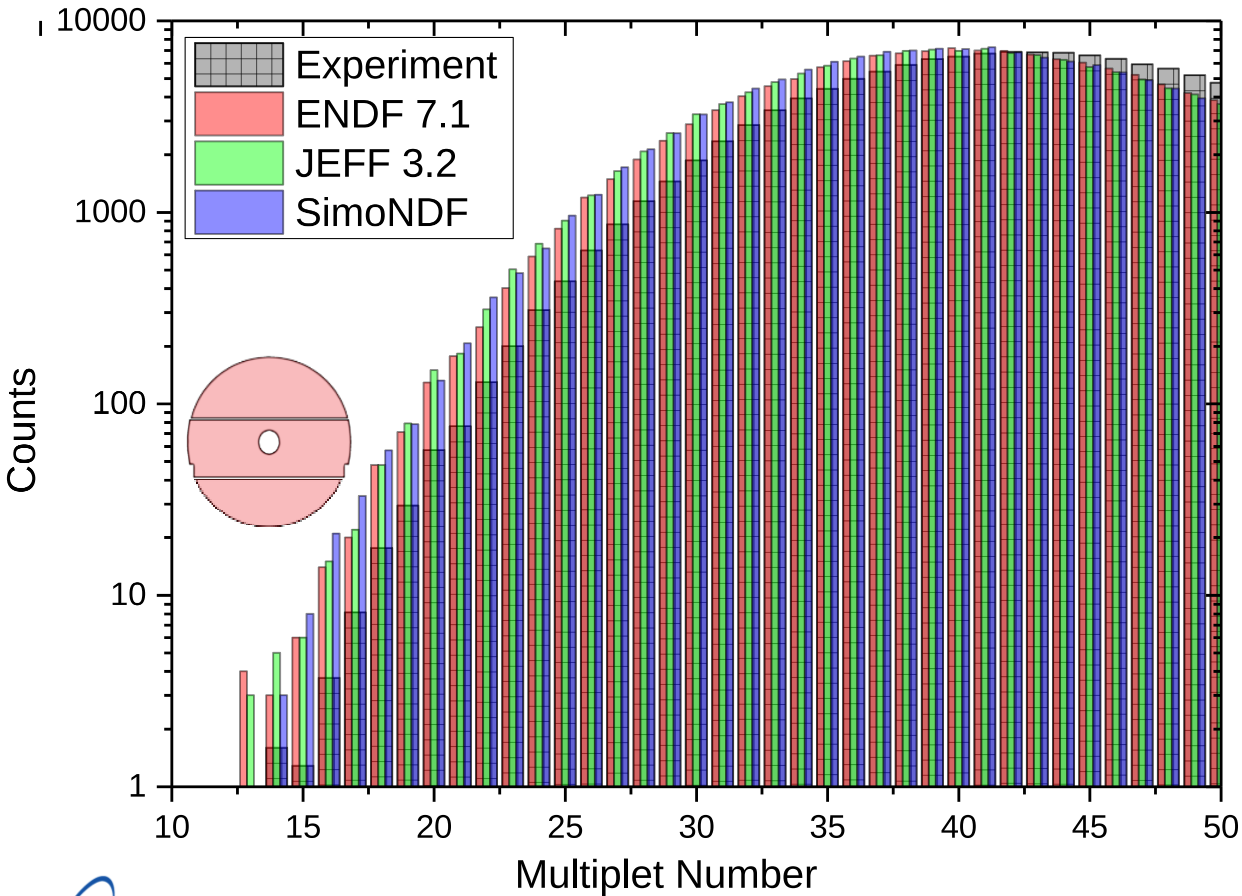
^{239}Pu Nuclear Data Library Comparisons

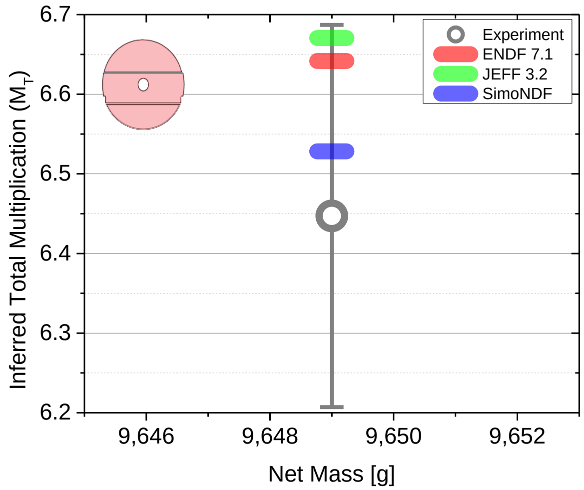




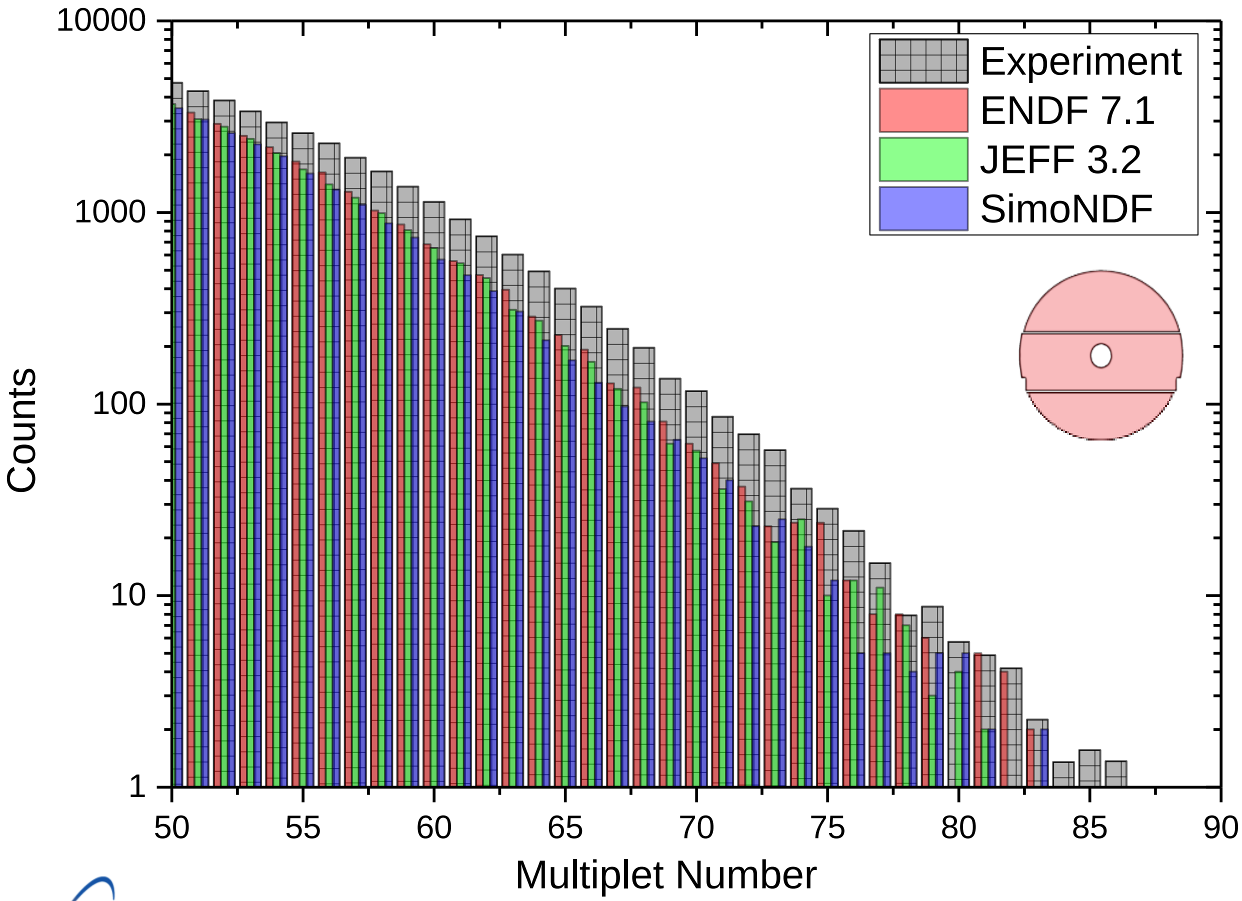
UNCLASSIFIED

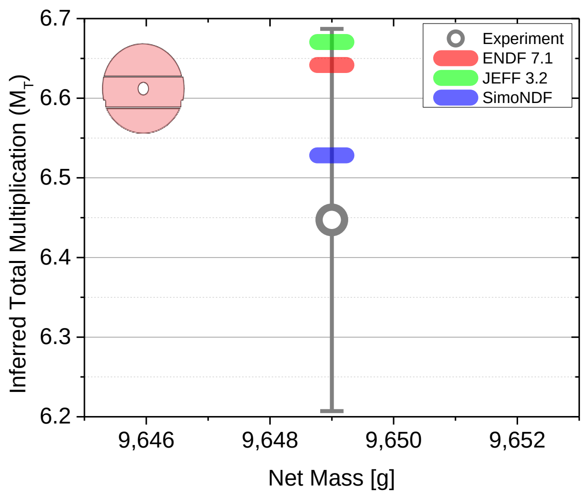
^{239}Pu Nuclear Data Library Comparisons





Nuclear Data Library Comparisons

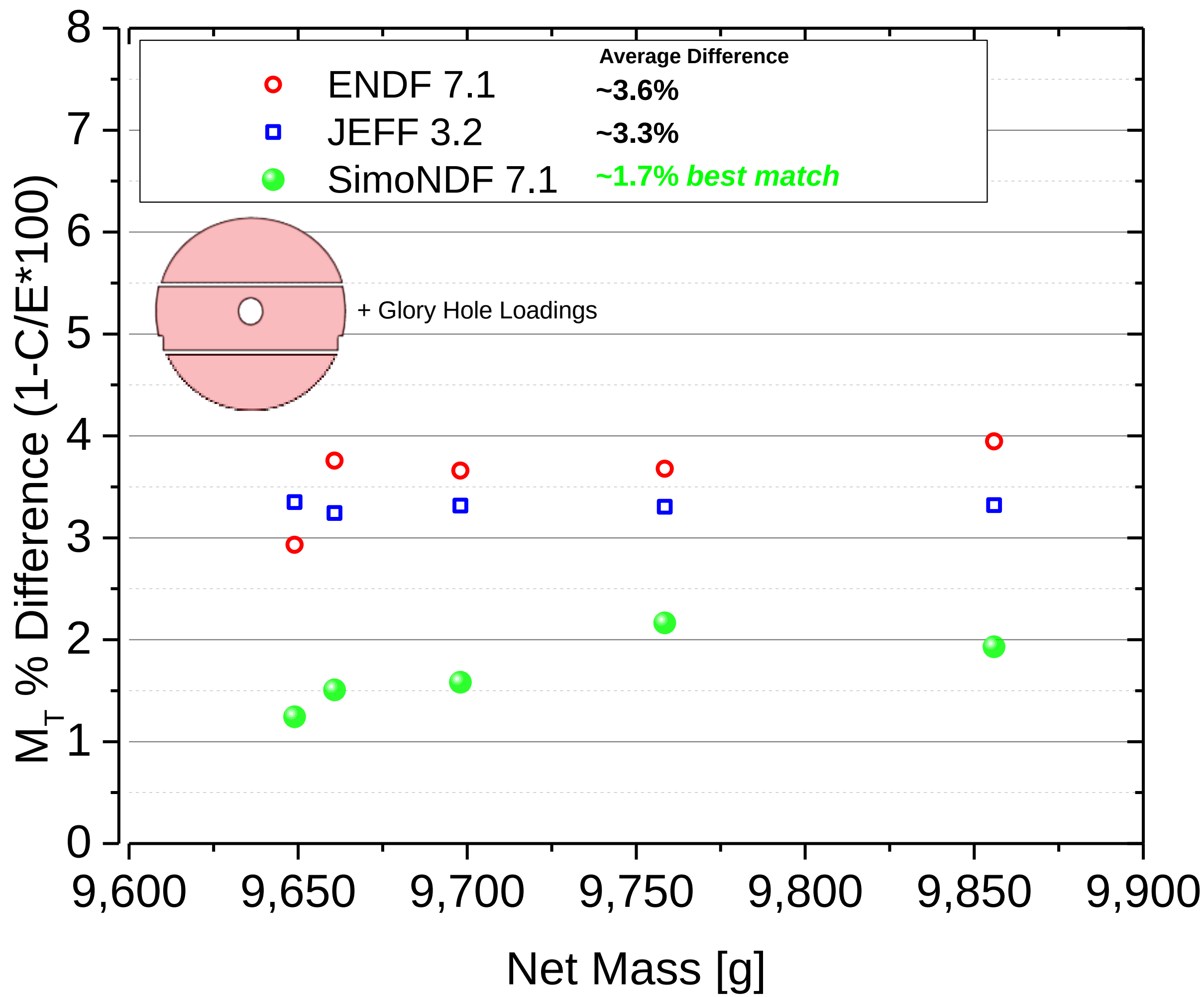




Nuclear Data Library Comparisons

Full assembly + loadings

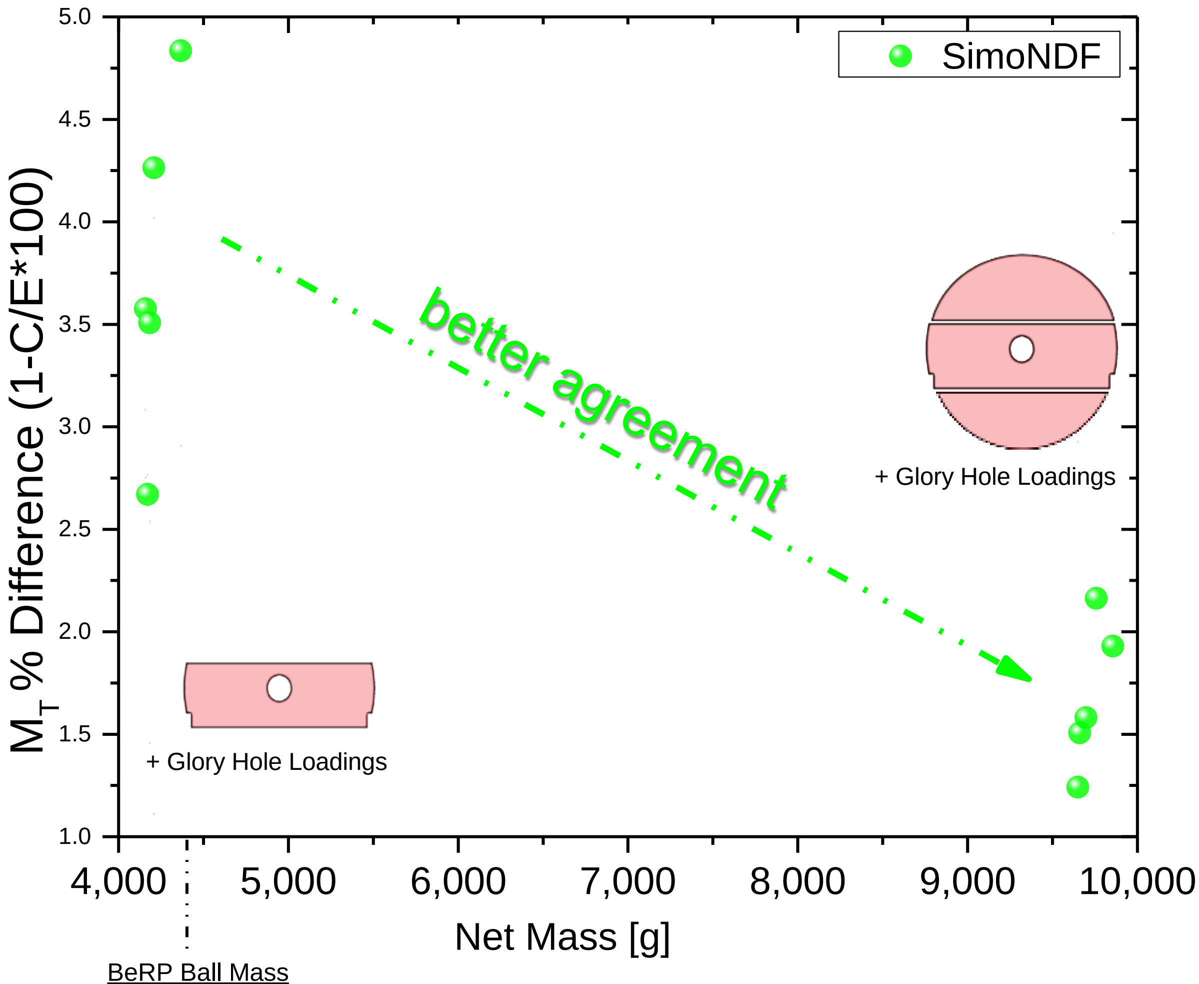
- "SimoNDF" is the clear best match.
- JEFF 3.2 is a slightly better match than ENDF 7.1.



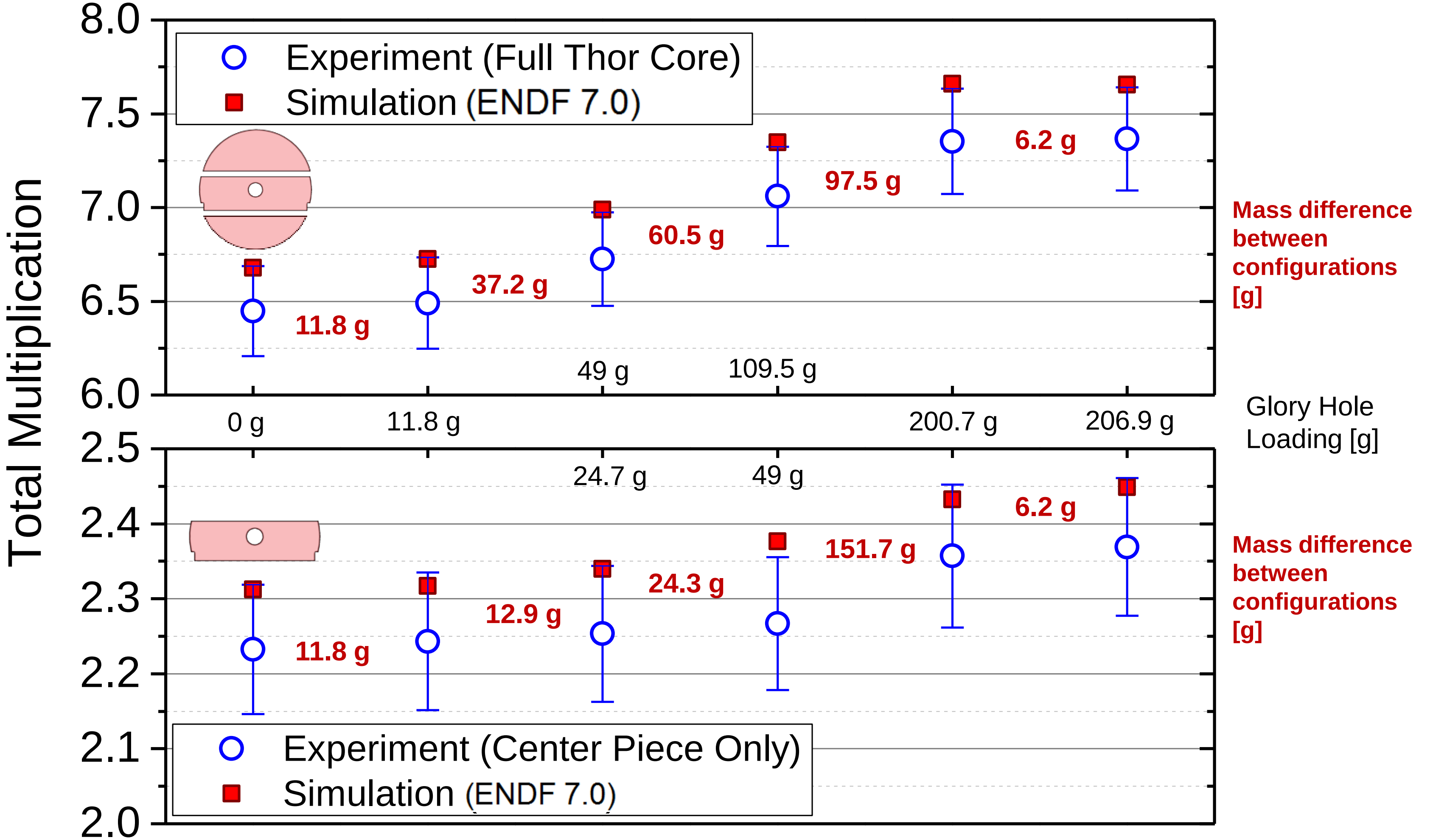
Nuclear Data Library Comparisons

Modified ENDF7.1 "SimoNDF"

- Correction to nubar based on BERP Ball (mass ~4500 g).
- Thor simulations with SimoNDF show better agreement at higher multiplication.

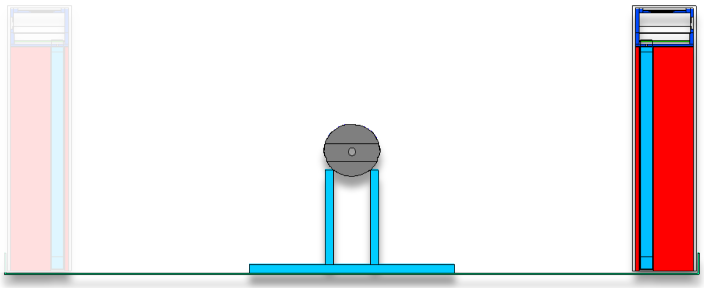


Detectable mass threshold decreases as mass (and system multiplication) increases.



Varying NPOD position provides an observable effect on the inferred neuron multiplication.

- **Varying the Source-to-Detector distance.**
  - Efficiency of stationary NPOD increases as varying NPOD moves closer.
- **Shifted NPOD (5 cm):**
  - Simulation: **27%** ↑ in R1, **75%** ↑ in R2
  - Experiment: **25%** ↑ in R1, **41%** ↑ in R2
- **Stationary NPOD:**
  - Simulation: **0.85%** ↑ in R1, **2.5%** ↑ in R2
  - Experiment: **0.94%** ↑ in R1, **2.5%** ↑ in R2
- **Removing NPOD**
  - – Presence of an NPOD adds reflection that another NPOD can see.
  - Simulation: **4.4%** ↑ in multiplication
  - Experiment: **3.9%** ↑ in multiplication



Deducing the possible sources of uncertainty/bias in the simulation results.

- **Underlying nuclear data**
  - Analysis of detector count rates of Pu-metal systems suggests that inferred subcritical multiplication is very sensitive to fast nubar of Pu-239.
- **Thor system specifications**
  - Geometry re-evaluation performed.
  - Isotopic composition.
- **Modeled NPOD efficiency**
  - Overestimate of gas pressure or active length could lead to higher inferred values*.
  - Improved efficiency measurements underway (for BeRP experiment with identical setup).
- **Radiation transport code**
  - Computational transport codes will always have some limitations.
  - MCNP6 expected to provide improved physics relative to this application.

E. C. Miller et al. "Computational Evaluation of Neutron Multiplicity Measurements of Polyethylene-Reflected Plutonium Metal," Nucl. Sci. and Eng. 176(2), 167-185 (2014).

R. Evans et al. "Sensitivity Analysis and Data Assimilation in A Subcritical Plutonium Metal Benchmark," Nucl. Sci. and Eng. 176(3), 325-338 (2014).

R. Evans, J. Li, J. Mattingly, "Adjoint Sensitivity Analysis in a Large-Scale Subcritical Plutonium Benchmark," Trans. of ANS 108, 487-490 (2013).

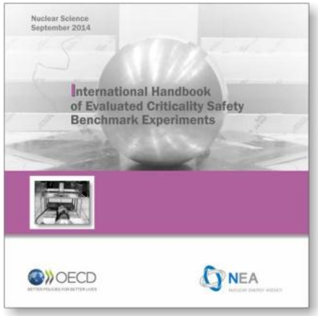
S. Bolding et al. "Simulations of Multiplicity Distributions with Perturbations to Nuclear Data," Trans. of ANS, 109, 251-254 (2013).

Comparing experiments and simulations helps in assessing/reducing uncertainties in models and data.

- **Ongoing effort to accurately quantify uncertainty in neutron multiplication inference from measurements and calculations.**

- **Significant improvements will depend on:**
  - Performing these types of measurements/simulations.
  - Proper documentation, for example:

> B. Richard, J. Hutchinson, “Nickel-Reflected Plutonium-Metal-Sphere Subcritical Measurements”
> Intl. Handbook of Evaluated Criticality Safety Benchmark Experiments
> NEA/NSC/DOC/(95)03/I, FUND-NCERC-PU-HE3-MULT-001(2014)



  - Incremental improvements in computational tools.
  - Leveraging community-wide parallel efforts related to quantifying uncertainties and correlations for nuclear data.
  - Applying new analyses techniques.
    - e.g. Bayesian interpretation of historical benchmark data.

Acknowledgements

- **This work was supported by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.**

UNCLASSIFIED

Questions?