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# Update for IER 489: Critical Unresolved Region Integral Experiment (CURIE)

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*March 2019*

*NCSP Technical Program Review*



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

## Outline

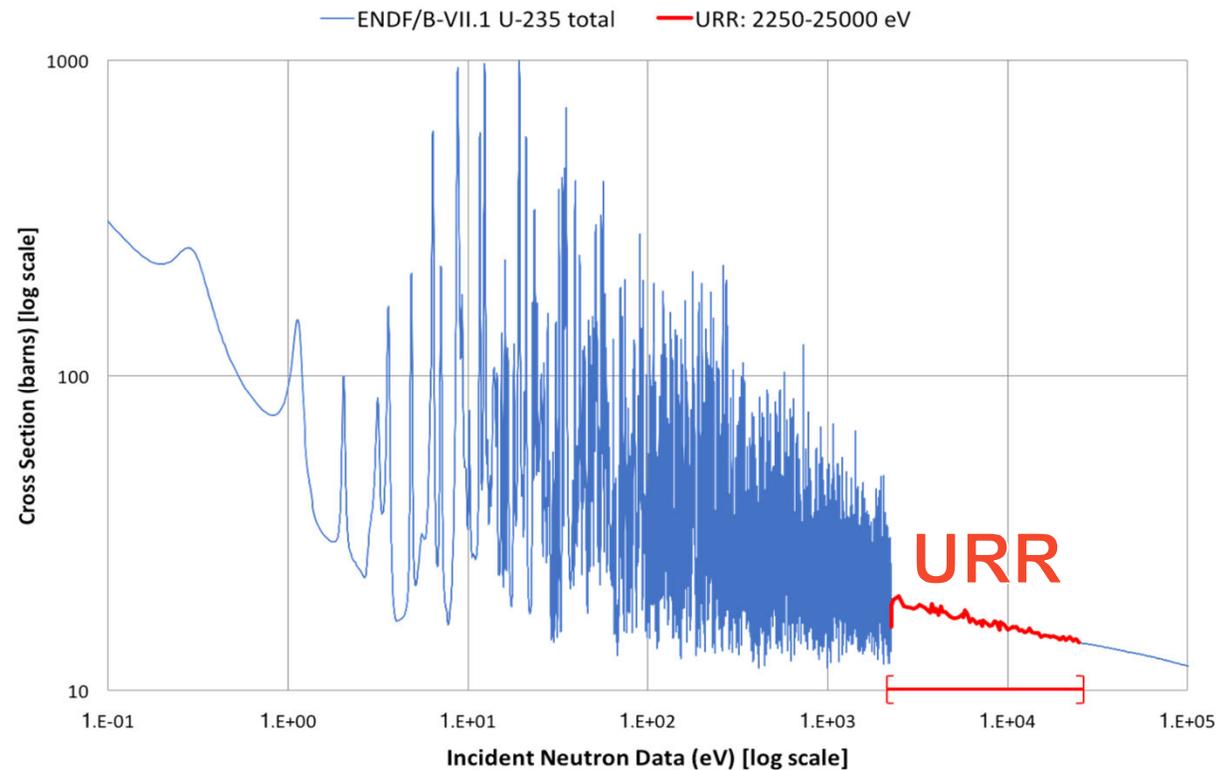
- What is the URR?
- Motivation
- Zeus Overview
- Assessment of Copper in Nuclear Data Libraries in Simulations
- CURIE Final Design
- Future Work



# Introduction

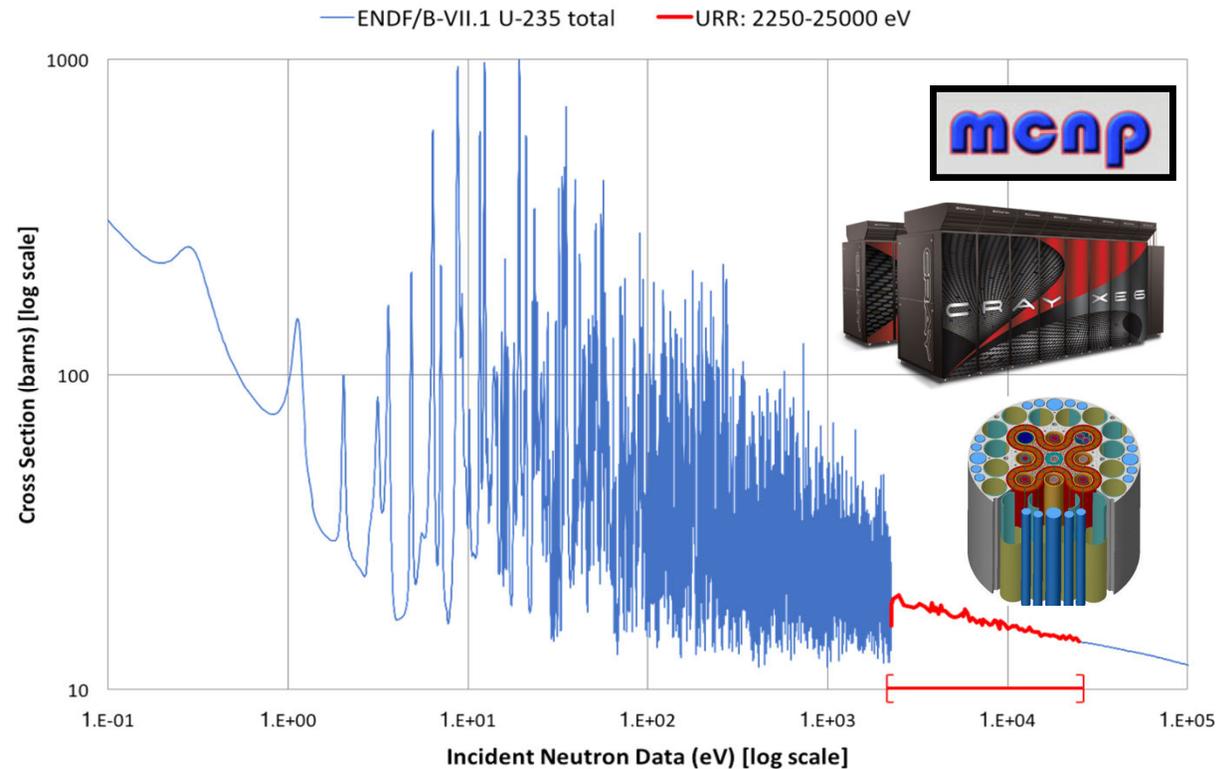
# Where is the Neutron Cross Section Unresolved Resonance Region (URR)?

- **The URR is generally located in the neutron cross section intermediate energy region**
  - The intermediate energy region is generally considered to be between 0.7 eV and 100 keV
- **The URR is specifically located after the resolved resonance region (RRR) ends, but before the fast (smooth) region begins**
  - There are distinct physical resonances at these energies, but they cannot be fully determined empirically.
  - URR is different for different isotopes and different data evaluations



# How is the URR currently being treated in Monte Carlo transport codes?

- In the URR, average resonance parameters extracted from experimental data are used to produce probability distribution functions (pdf) representing the total neutron cross section.
  - Mean value is the infinitely dilute smooth average of the cross section
- These distribution functions are represented in tabular form for application in MC transport codes and are referred to as “probability tables”.
  - “ladders” of sampled resonances based on average parameters and statistical laws
  - generated as a pre-processing step before the start of a simulation and are sampled at each instance that a URR cross section is needed.
  - more accurately represent the data to properly capture self-shielding effects

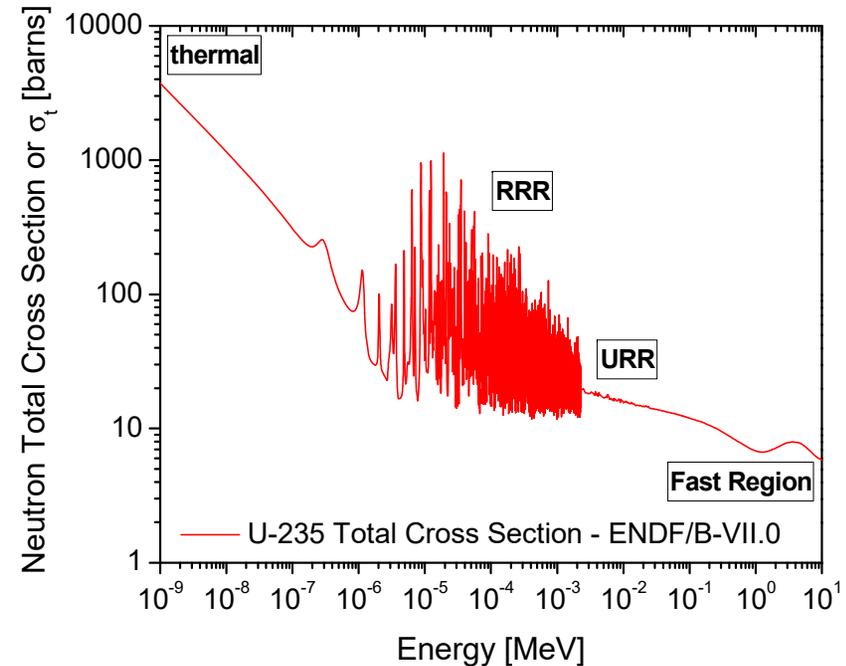


**Motivation**

# Why is the Unresolved Resonance Region for $^{235}\text{U}$ important to re-visit?

## #1: Differential Nuclear Data Validation

- **New US differential measurements**
  - New high resolution  $^{235}\text{U}$  capture measurements from RPI (Danon et al.) and LANL (Jandel et al.) were significantly below ENDF/B-VII.1 below 2 keV and above it for energies up to 50 keV
- **Recently updated ENDF/B-VIII.0  $^{235}\text{U}$  evaluated file incorporated changes in the capture cross section based on these measurements.**
- **There still remains disagreements between international evaluations**
  - URR bounds and average parameters
  - Additional evaluation work and new high-resolution capture data will be needed to improve the evaluated fission and capture cross sections in the energy region up to about 50 keV.



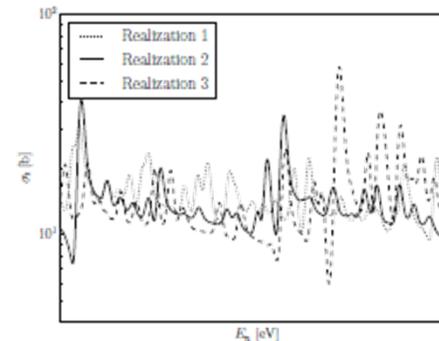
$^{235}\text{U}$  URR Bounds for Several Data Libraries

ENDF/B-VIII.0	2.25 keV - 25 keV
JEFF 3.2	2.25 keV - 25 keV
JENDL 4.0	500 eV - 30 keV

# Why is the Unresolved Resonance Region for $^{235}\text{U}$ important to re-visit?

## #2 Computational Methods Validation

1. As previously noted, production Monte Carlo codes have typically used the probability table method to account for self shielding in the URR
2. Recent work by Walsh et al. (MIT/LLNL) provides an alternative method by which a single resonance structure is realized and used throughout a single neutron transport simulation.
  - Used same sampling techniques as probability tables, but does not rely on a pre-processing step.
3. All URR methods implemented in Monte Carlo codes will benefit from additional benchmark experiments, such as CURIE



OpenMC

## Why is the Unresolved Resonance Region for $^{235}\text{U}$ important to re-visit?

### #3: Integral Benchmarks for URR Data and Methods Validation are Sparse

- **Only a handful of intermediate benchmarks available/used for the  $^{235}\text{U}$  evaluation in this region.**
  - ZEUS is used in all of them.
- **This is the first benchmark designed to focus specifically on URR as opposed to intermediate (in general).**
  - RPI is also exploring quasi-integral experiment designs for a dedicated complimentary set of  $^{235}\text{U}$  URR validation measurements of the URR.
- **Intermediate benchmark may help with other  $^{235}\text{U}$  nuclear data validation needs**
  - Intermediate energy benchmarks found to be sensitive nubar changes (See CSEWG presentation by A. Pavlou, J Thompson).

Naval Nuclear Laboratory Analysis of the  
ENDF/B-VIII.0 $\beta$ 5 Library

CSEWG 2017  
November 6-9, 2017

# Zeus Overview

# Zeus

- **Initially Designed and Conducted at the Los Alamos Critical Experiments Facility in mid 1990s**
  - Designed to address need for intermediate energy integral experiments
    - Established by criticality safety community
  - Considerations that factored into Zeus design
    - Requires large amount of SNM
    - Similarly, requires large overall size
    - Mid Z number reflector would reduce size and SNM quantity to within the LACEF inventory
    - Mid Z number reflector would return neutrons to core with some energy loss, but not overly thermalized
- **National Criticality Experiments Research Center located at the Nevada National Security Site**
  - Four critical assembly devices: Comet, Planet, Flat-Top, Godiva-IV
    - Zeus experiments have been reproduced here on Comet



# Zeus- General Description

- **HEU plates**

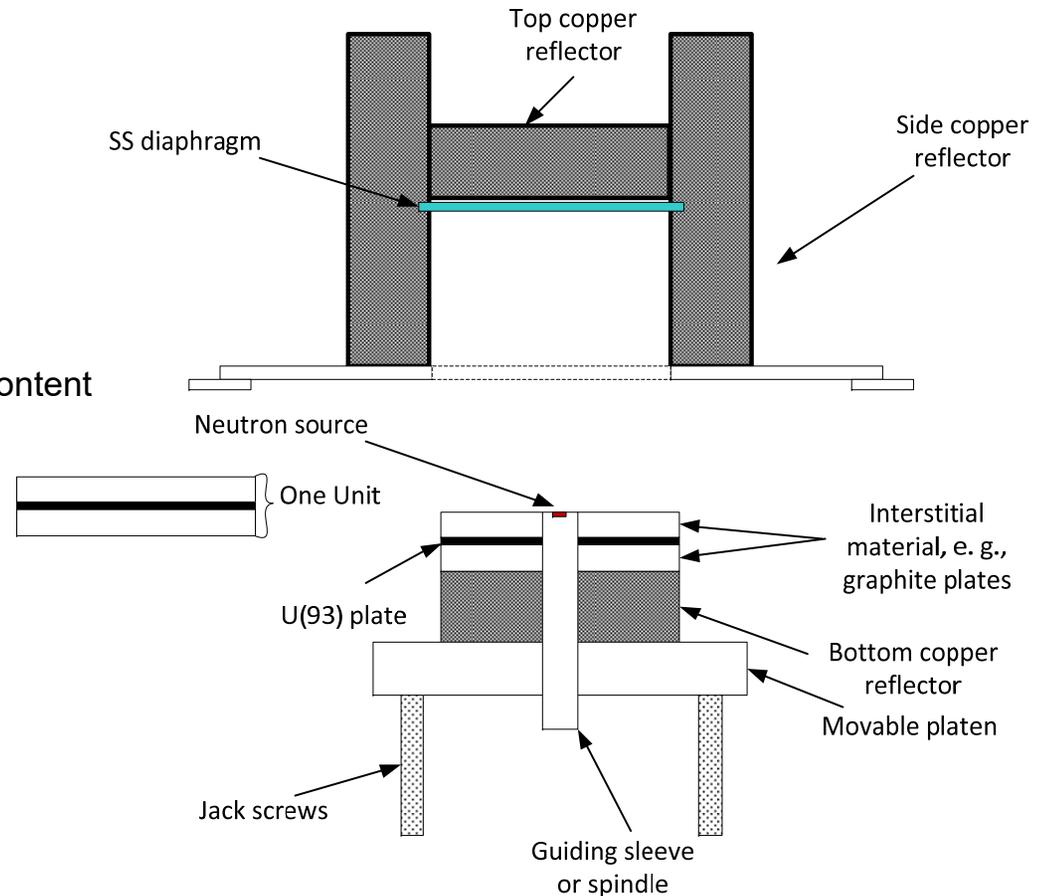
- 0.299 cm thick, 53.34 cm OD
- ~93 wt% U-235

- **Copper Reflector**

- 16.205 cm thick on all sides (including top and bottom)
- Log form to reduce leakage gaps
- All pieces are well characterized with known impurity content
- All at least 95 wt% Cu

- **Moderators**

- Varying amounts of plates of stock thickness
- Well-characterized
- Continuous Pattern
- Ex: graphite, iron, polyethylene, lead



# **Assessment of Copper in Nuclear Data Libraries in Simulations**

## Methods

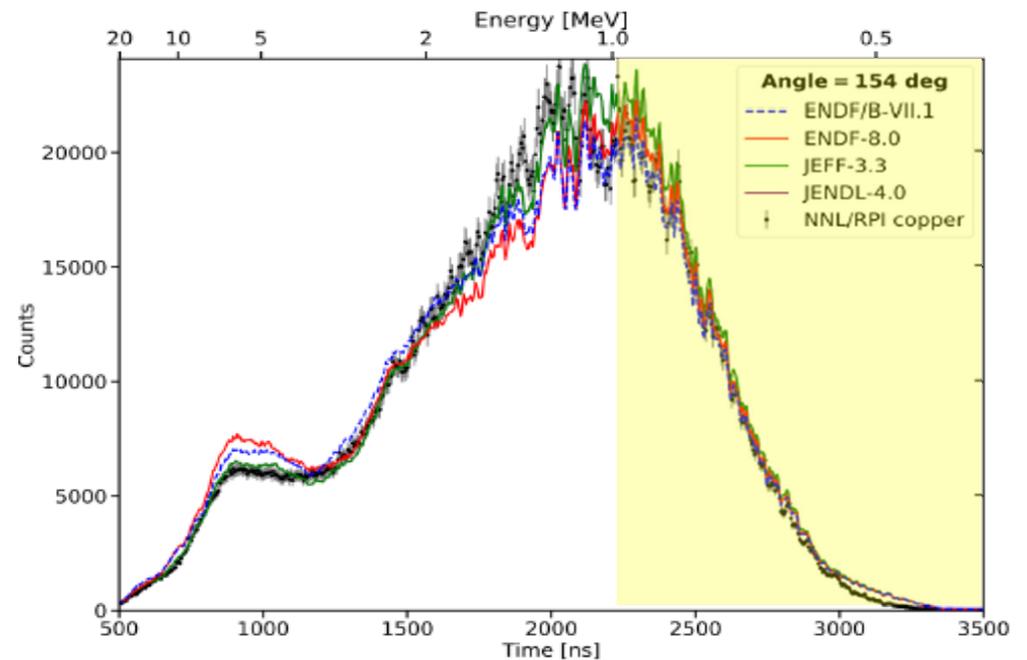
Comparisons between simulations and experiments have been discussed/ published/ presented at various nuclear data community events (CSEWG, NDAG, ANS etc..)

- Based on recent simulations of quasi-differential measurements of copper performed by D. Barry et. al.
- Also, based on past simulation results of integral experimental comparisons by L. Leal et al.
- Results from both exhibit typical (as opposed to outlier) differences and/or biases

# Recent Quasi-Integral Measurements at RPI

## High-energy-neutron-scattering experiments for copper from 0.5 to 20 MeV

- Analyzed using time of flight (TOF) technique with EJ301 detectors
- Results compared with high fidelity MC codes
- This technique has been well established at RPI to validate Zr, U, Fe, and other elements
  - Has also been transitioned to LANSCE

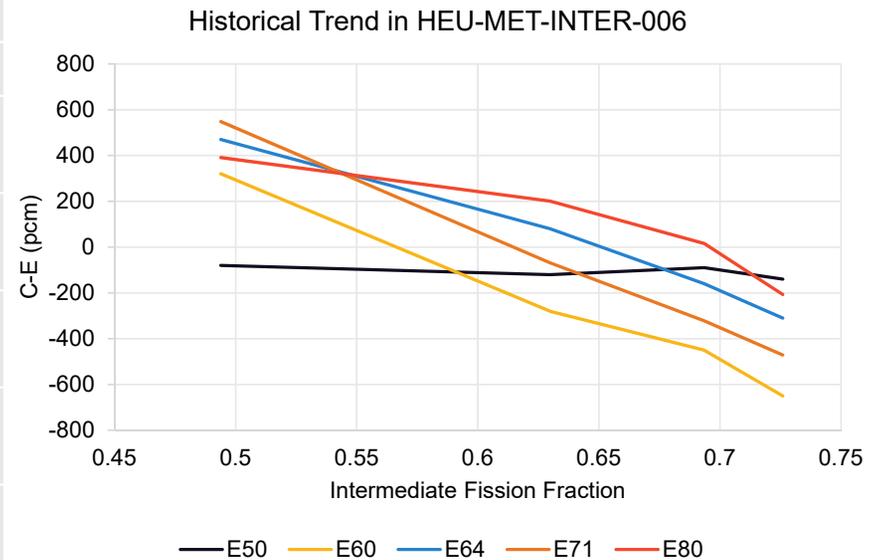


## Previous Integral Experiments

- Significant progress has been made on copper nuclear data isotopic evaluations
- Based on recent discussions with the primary evaluator of Copper in this region (Luiz Leal), Zeus was really the primary benchmark series used in the past few intermediate evaluations because of its average lethargy, high quality, and availability
- For ENDF/B-VIII.0, the pcm differences are consistent with differences observed in comparisons to other sets of integral ICSBEP experiments that are sensitive to other materials.
  - However, as pointed out by Mike Zerkle, there remains a trend in C/E vs. fission fraction that will continue to be explored

# Zeus Benchmark Results

ENDF Library	(C-E) [pcm]				
	V	VI	VI.4	VII.1	VIII
HEU-MET-FAST-073-001	-420	780	-	775	-65
HEU-MET-INTER-006-001	-140	-650	-310	-471	-207
HEU-MET-INTER-006-002	-90	-450	-160	-322	16
HEU-MET-INTER-006-003	-120	-280	80	-69	201
HEU-MET-INTER-006-004	-80	320	470	548	391



Benchmark results show overall improvement as cross sections are improved to better match the integral results and differential nuclear data.

Many experiments (differential and integral) have been done to support this effort.

# **CURIE Final Design**

# Preliminary Design: Critical Unresolved Region Integral Experiment (CURIE)

- **National Criticality Experiments Research Center located at the Nevada National Security Site**

- Extensive SNM inventory
- Four critical assembly devices: Comet, Planet, Flat-Top, Godiva-IV

- **Zeus is a good starting point**

- Used in most recent  $^{235}\text{U}$  URR Evaluation(s)
- Assembly reflector/interstitials exist/easily accessible
- Recent Zeus measurements at NCERC performed with Pb

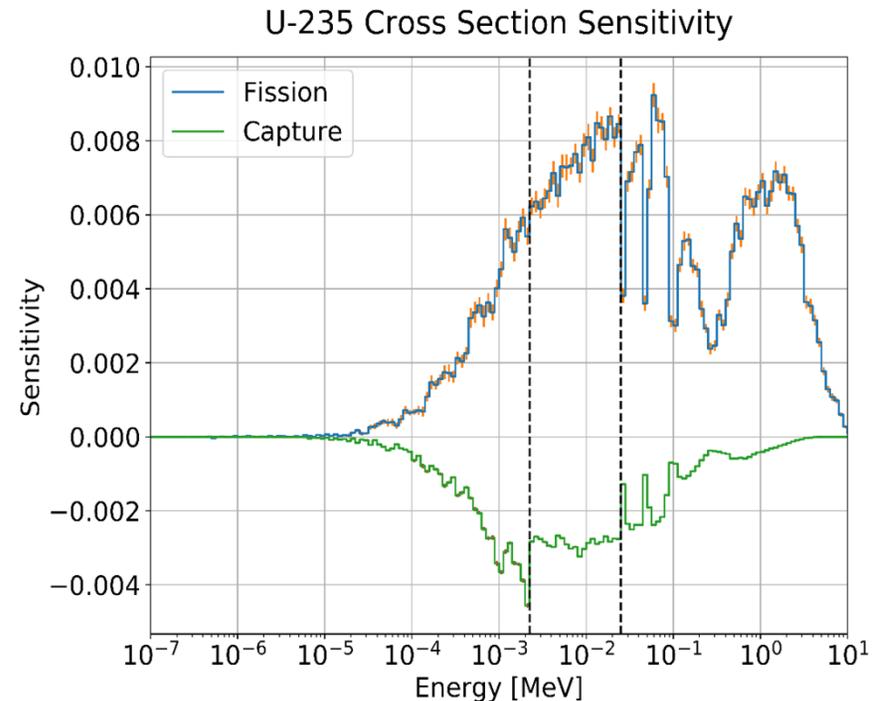
- **CURIE is the next step**

- **Critical Unresolved Region Integral Experiment (CURIE)**
- Final Design
  - Based on preliminary design (CED-1)
  - Utilized optimization techniques and physics-based approach
  - Parameters considered:
    - Reflector, moderator, and fuel
      - » Material and thickness



# Final Design: Critical Unresolved Region Integral Experiment (CURIE)

- **Zeus setup (same HEU plates, same copper reflector)**
- **Moderators considered**
  - Lucite, Teflon, BeO, Be, Graphite, Alumina
  - Optimized thickness for fission sensitivity in the URR
- **Utilized ENDF-B/VII.1 and MCNP®6.2**
- **Additional Parameters of Interest**
  - URR Capture Sensitivity
  - Total Fission Integral Sensitivity
  - Fission to Capture Ratio Integral Sensitivity
  - URR Fission to Capture Ratio Integral Sensitivity
  - Financial Feasibility



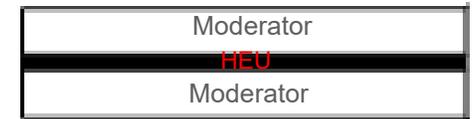
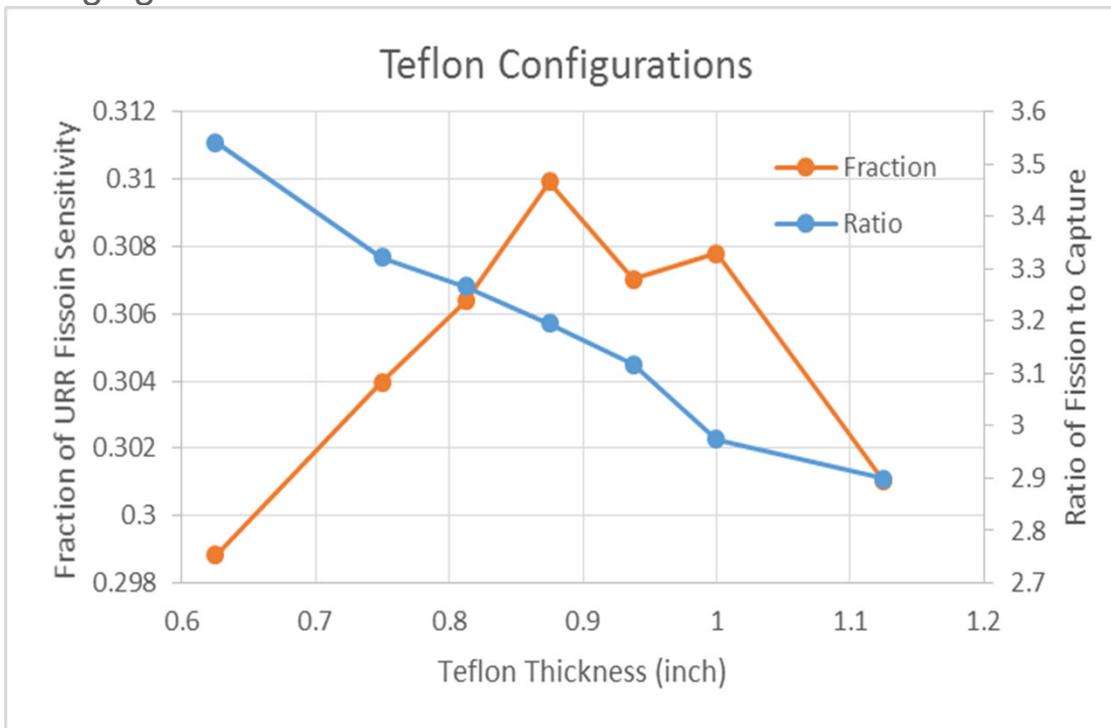
# Final Design: Critical Unresolved Region Integral Experiment (CURIE)

Material	Lucite	BeO	Be	HMI006-3	Graphite	Alumina	Teflon
Thickness [cm]	0.466	1.677	1.135	2.015	1.640	2.011	2.276
<b>URR Fission Sensitivity Fraction</b>	0.1027	0.2027	0.2096	0.2173	0.2202	0.2844	0.3087
URR Capture Sensitivity Fraction	0.0452	0.1007	0.0837	0.0906	0.0912	0.1074	0.1178
Total Fission Sensitivity Integral	0.4051	0.4143	0.4794	0.4889	0.4973	0.5104	0.4967
Total Capture Sensitivity Integral	0.1829	0.1980	0.1689	0.1550	0.1458	0.1418	0.1575
Fission Integral to Capture Integral	2.21	2.09	2.84	3.15	3.41	3.60	3.15
URR Fission Integral to Capture Integral	2.27	2.01	2.50	2.40	2.41	2.65	2.62
Rating	Poor	Ok	Ok	Ok	Good	Better	Great

# Final Design: Critical Unresolved Region Integral Experiment (CURIE)

- **Final Selection**

- Teflon moderator plates
- Thicknesses ranging from 5/8" to 9/8"



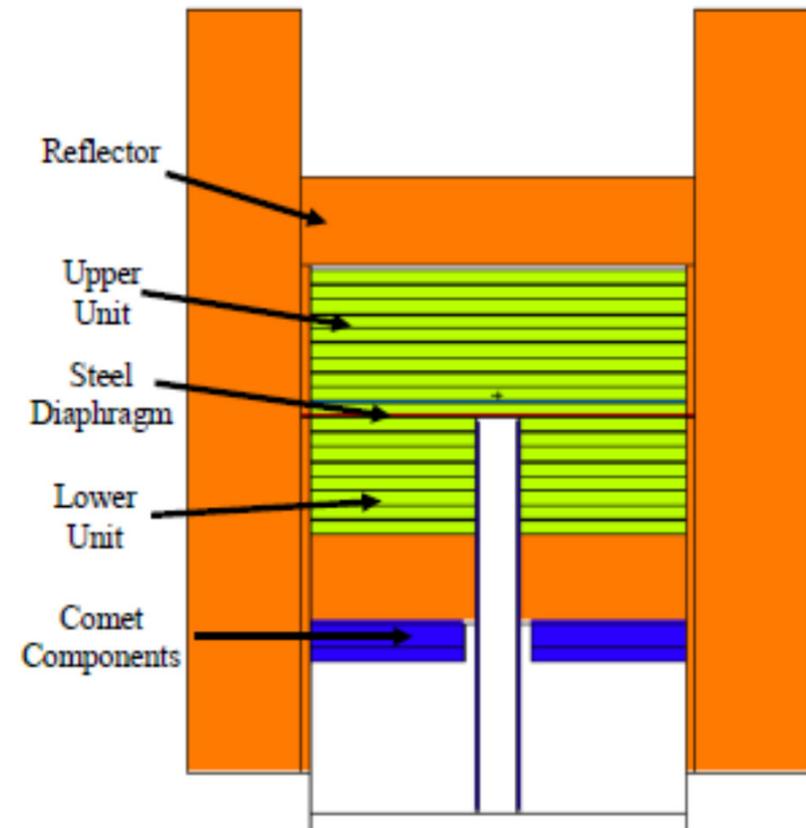
One Unit Cell

# Final Configurations

## • Final Selection

- Teflon moderator plates thickness
- Spans above and below the URR
- Setup for feasible and reproducible experiment design while maximizing use of components
- All expected to go critical with 9-10 units

Teflon Thickness (inch)	Unit Cell Pieces	$k_{\text{eff}}$
5/8	$2*(1/16'' + 1/4'')$	1.01463
6/8	$2*(1/8'' + 1/2'')$	1.00965
7/8	$2*(1/16''+1/8''+1/4'')$	1.00418
1	$2*(1/2'')$	1.02260
9/8	$2*(1/2'' + 1/8'')$	1.01399



## **Conclusions and Future Work**

## Future Work: CED-3a Work

- **Procure Teflon**
  - Assume 14 units is bounding need
  - Buy plates in thicknesses that allows them to be used for multiple configuration
- **Procure Diaphragm for Upper Portion of Stack**
  - Not needed; current membrane for Zeus experiments meets the needs and weight requirements
- **Update Experiment Plan**
  - Not needed; falls under currently approved Zeus Experiment Plan
- **Complete Additional Sensitivity Calculations**
  - This is to support the understanding of the URR effects during this experiment and thus aid in the CED-4 analysis

## Conclusions

- Moved from preliminary to final design for IER 489 - CURIE (Critical Unresolved Region Integral Experiment)
- The final design builds on the successful Zeus Intermediate Energy Range experiments with U-235, but focuses on the narrower Unresolved Resonance Region
- The final design relied on physics-based optimization methods
- CURIE CED 3a requirements are modest
- CURIE promises to add to the sparse suite of integral benchmarks to validate U-235 URR nuclear data and Monte Carlo transport methods

# Acknowledgments

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



**Backup**

## BACKUP: ENDF File for URR

Pointed out by Dave Brown for  $^{235}\text{U}$  :

Infinitely dilute cross-sections calculated from the average resonance parameters in ENDF file 2 is not always in agreement with the infinitely diluted cross section in file 3 (obtained from the best combination of measurements and models as provided by evaluators).

One can enforce the LSSF=1 option and adopt resonance parameter interpolation instead of cross section interpolation in the URR for more accuracy even though interpolating the cross section is a faster calculation.

## **BACKUP: Why can't we just measure the resonances in the URR?**

- **When the level spacing between isolated resonances becomes comparable to the average natural width of these resonances, a continuum of overlapping averaged resonances will be observed.**

## ZEUS + $^{235}\text{U}$ Unresolved Region Evaluation (2004)

L. Leal et al. "An Unresolved Resonance Evaluation for  $^{235}\text{U}$  " PHYSOR (2004)

<https://www.ipen.br/biblioteca/cd/physor/2004/PHYSOR04/papers/93492.pdf>

**Table 4** Comparisons of  $k_{eff}$  calculations using the unresolved  $^{235}\text{U}$  evaluation.

Benchmark	Experimental $k_{eff}$	MCNP ENDF66	MCNP ENDF66 with $^{235}\text{U}$ ORNL Evaluation
ORNL10	$1.0015 \pm 0.0010$	$0.9987 \pm 0.0004$	$0.9991 \pm 0.0004$
HISS/HUG	$1.0000 \pm 0.0040$	$1.0099 \pm 0.0005$	$1.0092 \pm 0.0005$
UH <sub>3</sub> (1)	$1.0000 \pm 0.0047$	$1.0040 \pm 0.0050$	$1.0020 \pm 0.0005$
Zeus (1)	$0.9976 \pm 0.0008$	$0.9918 \pm 0.0003$	$0.9899 \pm 0.0003$
Zeus (2)	$0.9997 \pm 0.0008$	$0.9945 \pm 0.0003$	$0.9927 \pm 0.0003$
Zeus (3)	$1.0010 \pm 0.0009$	$0.9990 \pm 0.0003$	$0.9965 \pm 0.0003$
Godiva	$1.0000 \pm 0.0010$	$0.9966 \pm 0.0001$	$0.9964 \pm 0.0001$

# ZEUS + <sup>235</sup>U Intermediate Energy Capture Evaluation (2004)

O. Iwamoto et al. “<sup>235</sup>U Capture Cross Section in the keV to MeV Energy Region” NEA/WPEC Subgroup 29 Final Report (2011)

[https://www.oecd-nea.org/science/wpec/meeting2011/Sg29\\_report-20110420.pdf](https://www.oecd-nea.org/science/wpec/meeting2011/Sg29_report-20110420.pdf)

Table 2. Energy of the average lethargy causing fission (AVG)

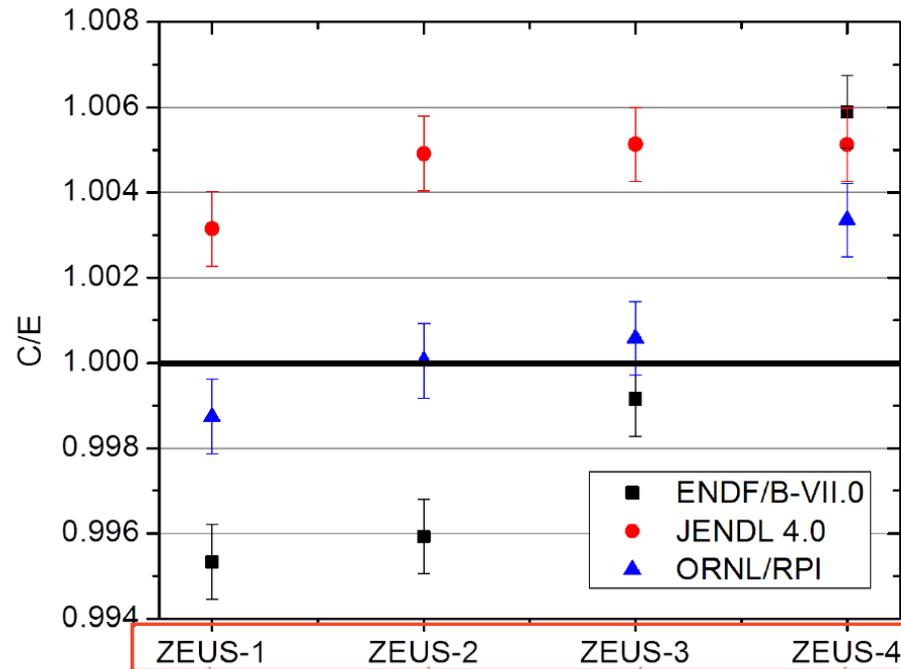
Name	Spectrum	Handbook ID	AVG (keV)	Case # (base)	500 eV	2250 eV	25.0 keV	30 keV
					RR	RR	URR	File 3
					RR	RR	URR	URR
ZEUS1	Intermediate	HEU-MET-INTER-006, case1	5.05	2	RR	URR	URR	URR
ZEUS2	Intermediate	HEU-MET-INTER-006, case2	10.33	3	RR	URR	URR	File 3
ZEUS3	Intermediate	HEU-MET-INTER-006, case3	24.02	4	RR	RR	URR	File 3
ZEUS4	Intermediate	HEU-MET-INTER-006, case4		5	RR	URR	URR	File 3
FCA-IX-1	Intermediate		29.90	6	RR	RR	URR	File 3
FCA-IX-2	Intermediate		116.52	7	RR	RR	URR	File 3
FCA-IX-3	Intermediate		211.30	8	RR	URR	URR	URR

LEGEND:

- ENDF/B-VII
- JENDL-3.2
- ENDF/B-VII (-3%  $\Gamma_g$ )
- ENDF/B-VII (-10%  $\Gamma_g$ )
- JENDL/AC-2008 URR

# ZEUS + $^{235}\text{U}$ Intermediate Energy Capture Evaluation (2014)

L. Leal et al. "Nuclear Data Evaluation Accomplishments" NCSP Program Review (2014)  
<https://ncsp.llnl.gov/TPRAgendas/2014/LEAL.pdf>



# Final Design: Critical Unresolved Region Integral Experiment (CURIE)

## Final Selection

- Teflon moderator plates
- Thicknesses ranging from 0.50 to 1.25 inches

Teflon Thickness (inch)	Unit Cells	$k_{\text{eff}}$
5/8	8	0.97644
5/8	9	1.01463
6/8	8	0.97490
6/8	9	1.00965
13/16	8	0.97334
13/16	9	1.00703
7/8	9	1.00418
15/16	9	1.00127
1	9	0.99805
1	10	1.02260
9/8	9	0.99143
9/8	10	1.01399

