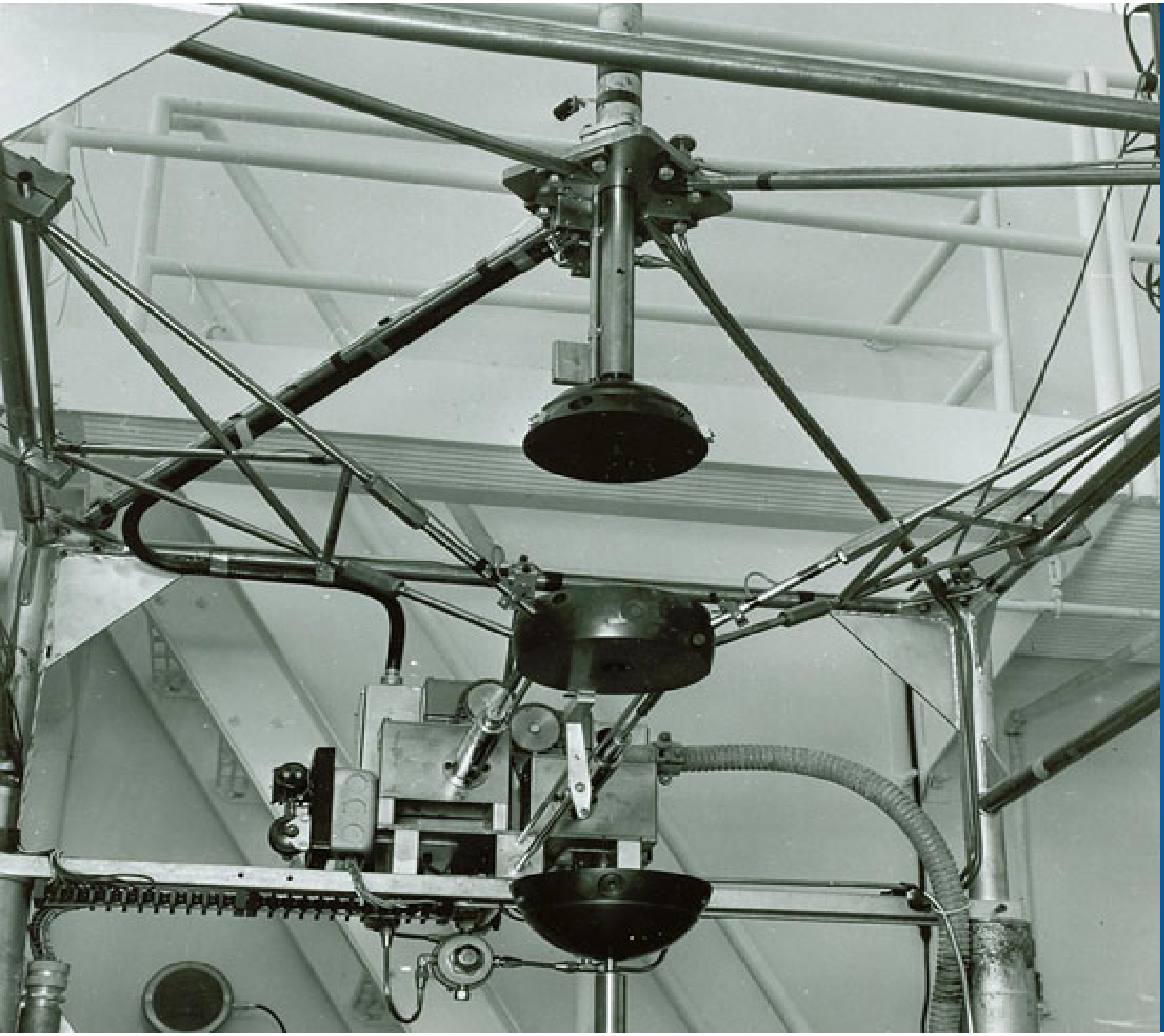

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Final Design of an Intermediate Energy Critical Experiment

for Validation of ^{235}U Unresolved Resonance Region Nuclear Data and Computational Methods

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

Outline

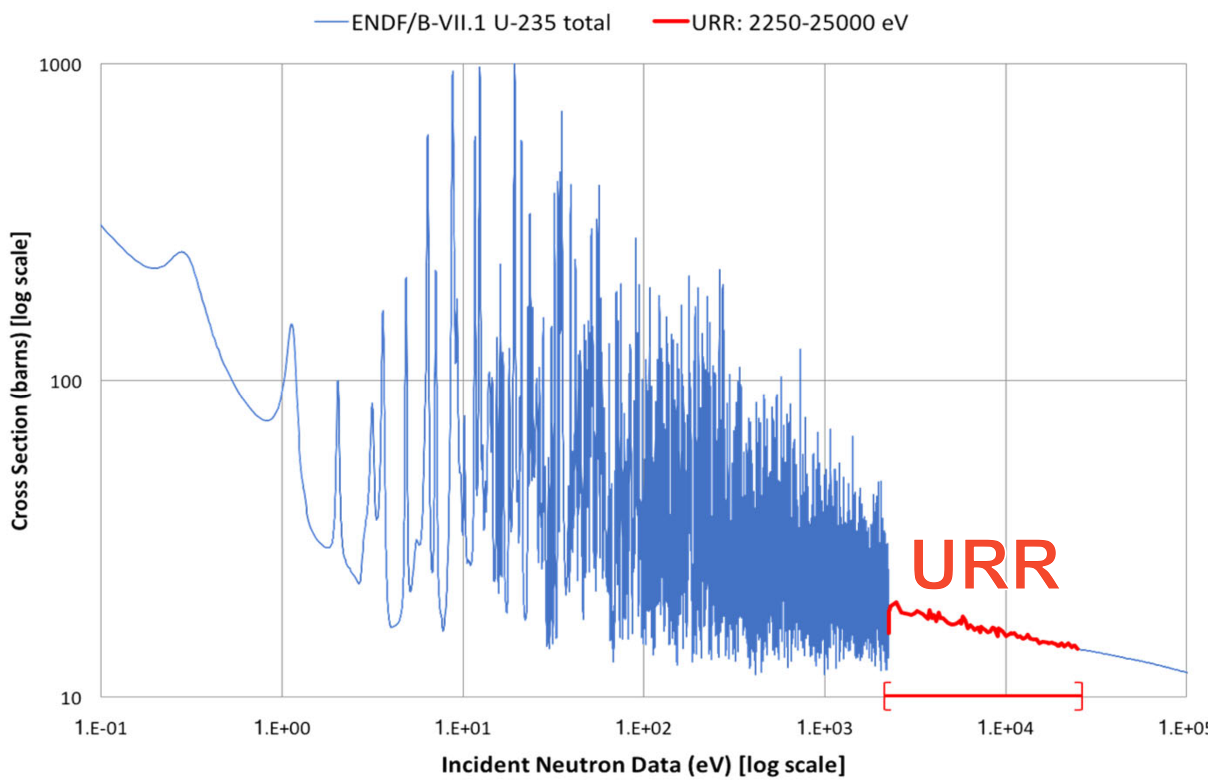
- What is the URR?
- Motivation
- Zeus Overview
- CURIE Final Design
- Future Work

Introduction

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

- **The URR is generally located in the neutron cross section intermediate energy region**
  - Defined as 0.7 eV to 100 keV

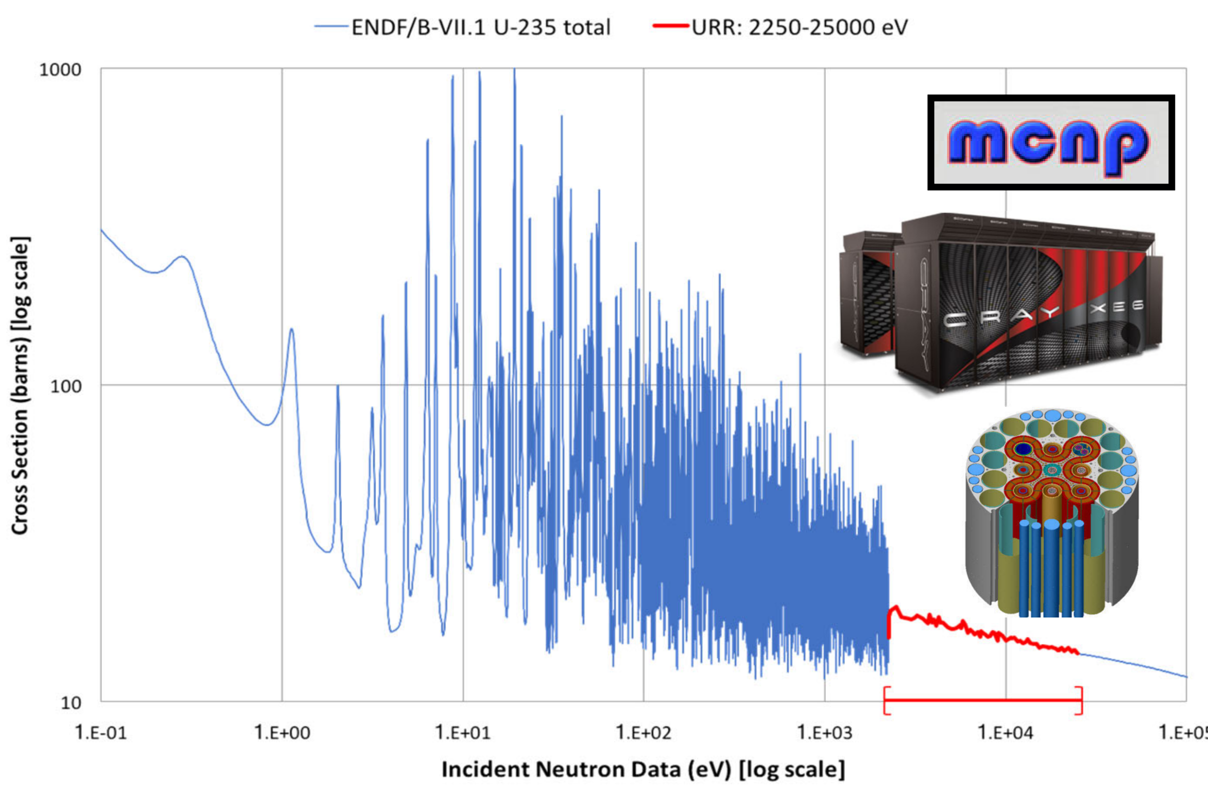
- **The URR is specifically located after the resolved resonance region (RRR) ends, but before the fast (smooth) region begins**
  - There are distinct physical resonances at these energies, but they cannot be fully determined empirically.



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

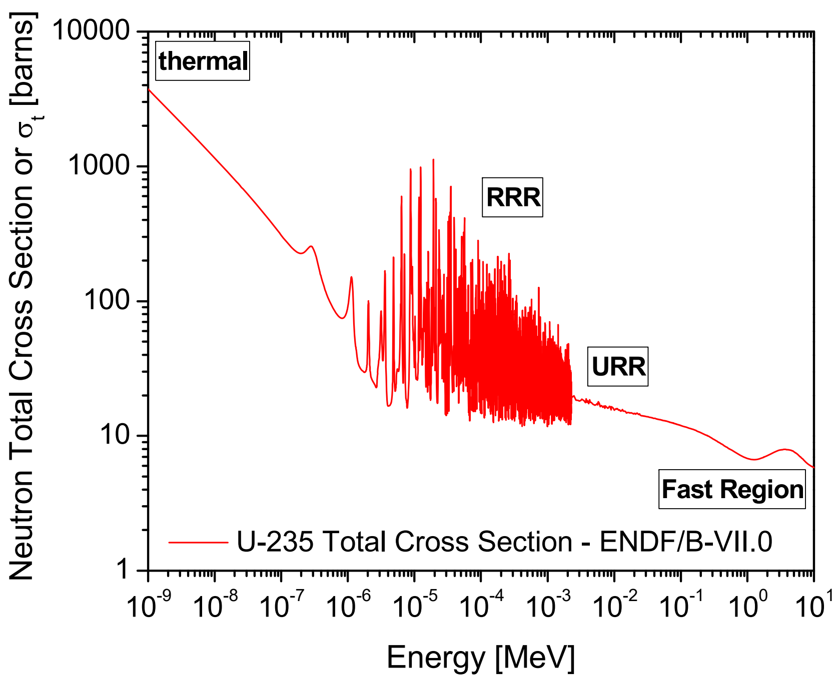


Motivation

Why is the Unresolved Resonance Region for 235U important to re-visit?

#1: Differential Nuclear Data Validation

- **New US differential measurements**
  - New high resolution ^{235}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 ^{235}U evaluated file incorporated changes in the URR based on new measurements.**
  - New ENDF evaluation incorporated capture measurements among other changes to the ^{235}U evaluated file.
- **There still remains disagreements between international evaluations**
  - URR bounds and average parameters.



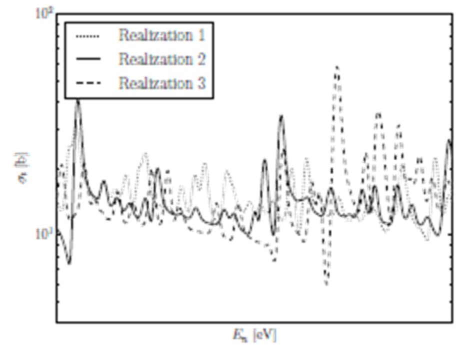
^{235}U URR Bounds for Several Data Libraries

ENDF/B-VII.1	2.25 keV - 25 keV
JEFF 3.2	2.25 keV - 25 keV
JENDL 4.0	500 eV - 30 keV

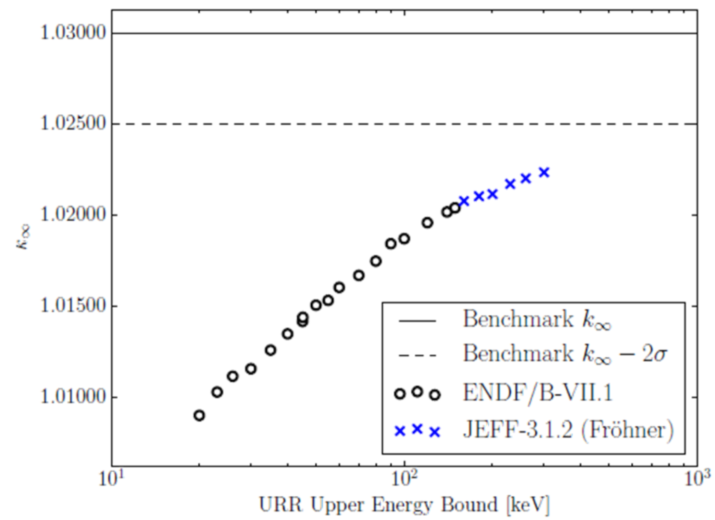
Why is the Unresolved Resonance Region for 235U important to re-visit?

#2 Computational Methods Validation Needs

- **Recent On-The-Fly Implementation of URR in MC transport codes**
  - 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.
  - More physical representation as it preserves the relationships between neighboring cross sections and uses the same cross section value for subsequent events at the same energy.
  - Can be used to quickly evaluate URR bound effect on criticality calculations e.g. Walsh et al. compared ZEBRA-8H prediction with different ^{235}U URR bounds.



OpenMC



ZEUS + ^{235}U Unresolved Region Evaluation (2004)

L. Leal et al. "An Unresolved Resonance Evaluation for ^{235}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}U evaluation.

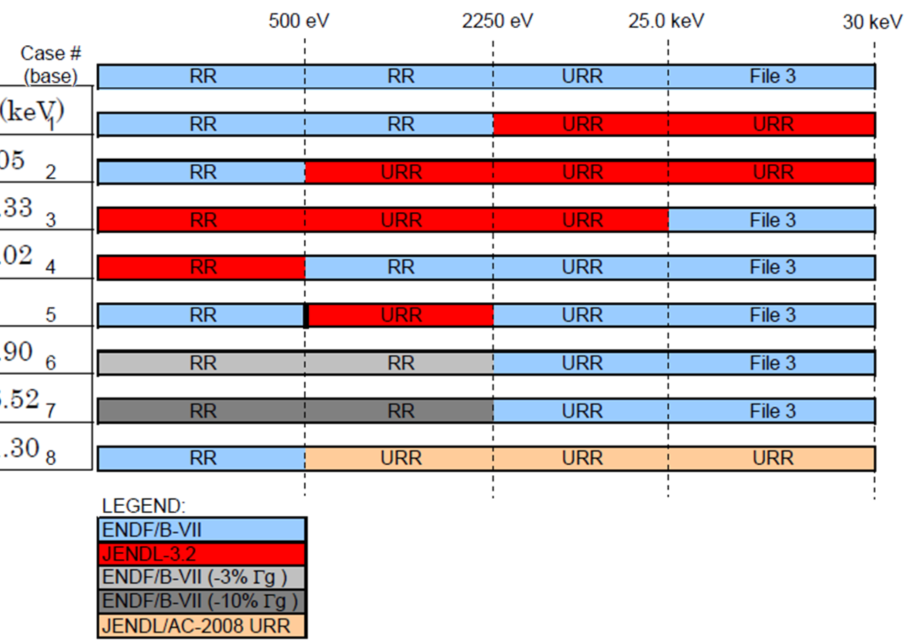
Benchmark	Experimental k_{eff}	MCNP ENDF66	MCNP ENDF66 with ^{235}U ORNL Evaluation
ORNL10	1.0015 ± 0.0010	0.9987 ± 0.0004	0.9991 ± 0.0004
HISS/HUG	1.0000 ± 0.0040	1.0099 ± 0.0005	1.0092 ± 0.0005
UH_3 (1)	1.0000 ± 0.0047	1.0040 ± 0.0050	1.0020 ± 0.0005
Zeus (1)	0.9976 ± 0.0008	0.9918 ± 0.0003	0.9899 ± 0.0003
Zeus (2)	0.9997 ± 0.0008	0.9945 ± 0.0003	0.9927 ± 0.0003
Zeus (3)	1.0010 ± 0.0009	0.9990 ± 0.0003	0.9965 ± 0.0003
Godiva	1.0000 ± 0.0010	0.9966 ± 0.0001	0.9964 ± 0.0001

ZEUS + ^{235}U Intermediate Energy Capture Evaluation (2004)

O. Iwamato et al. "^{235}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

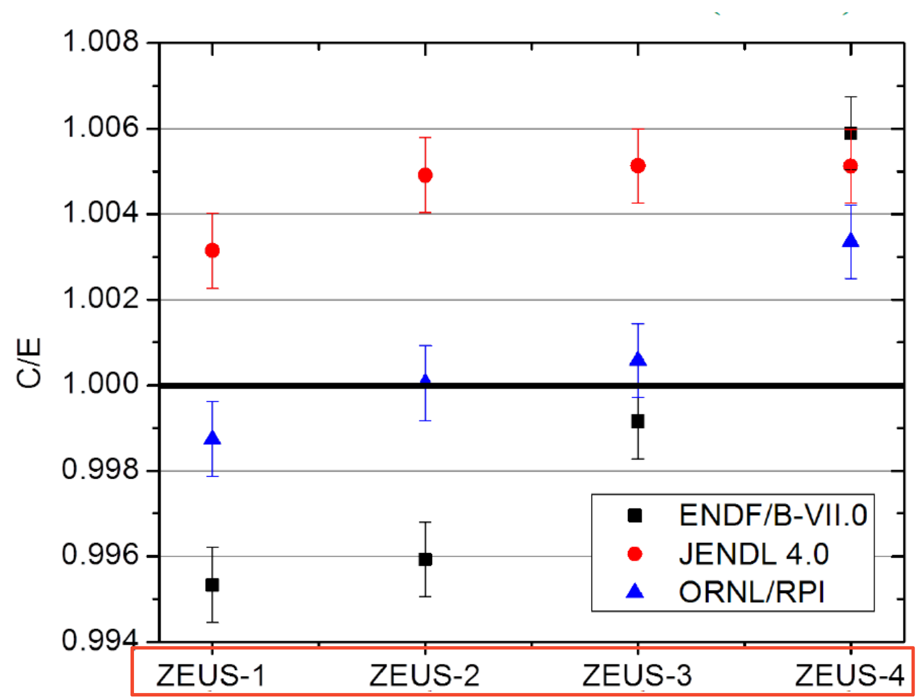
Table 2. Energy of the average lethargy causing fission (AVG)

Name	Spectrum	Handbook ID	AVG (keV)
ZEUS1	Intermediate	HEU-MET-INTER-006, case1	5.05
ZEUS2	Intermediate	HEU-MET-INTER-006, case2	10.33
ZEUS3	Intermediate	HEU-MET-INTER-006, case3	24.02
ZEUS4	Intermediate	HEU-MET-INTER-006, case4	
FCA-IX-1	Intermediate		29.90
FCA-IX-2	Intermediate		116.52
FCA-IX-3	Intermediate		211.30



ZEUS + ^{235}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



Why is the Unresolved Resonance Region for ^{235}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}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}U URR validation measurements of the URR.
- **Intermediate benchmark may help with other ^{235}U nuclear data validation needs**
  - Intermediate energy benchmarks found to be sensitive nubar changes (See CSWEG presentation by A. Pavlou, J Thompson).

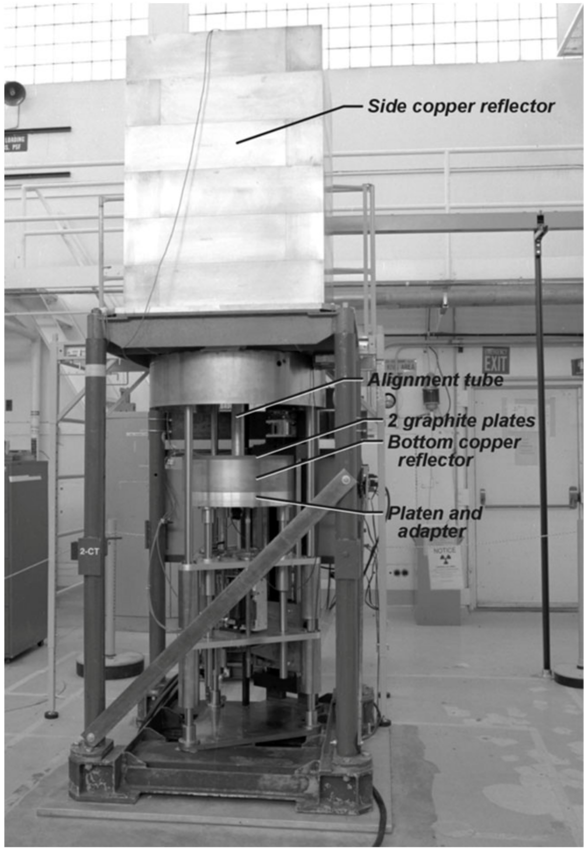
Naval Nuclear Laboratory Analysis of the ENDF/B-VIII.0β5 Library
CSEWG 2017
November 6-9, 2017

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
  - Known facts about planned system
    - Requires large amount of SNM
    - Similarly, requires large overall size
    - Moderate reflector would reduce size and SNM quantity to within the LACEF inventory
    - Moderate 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 is a good starting point**
  - Used in most recent ^{235}U URR Evaluation(s)

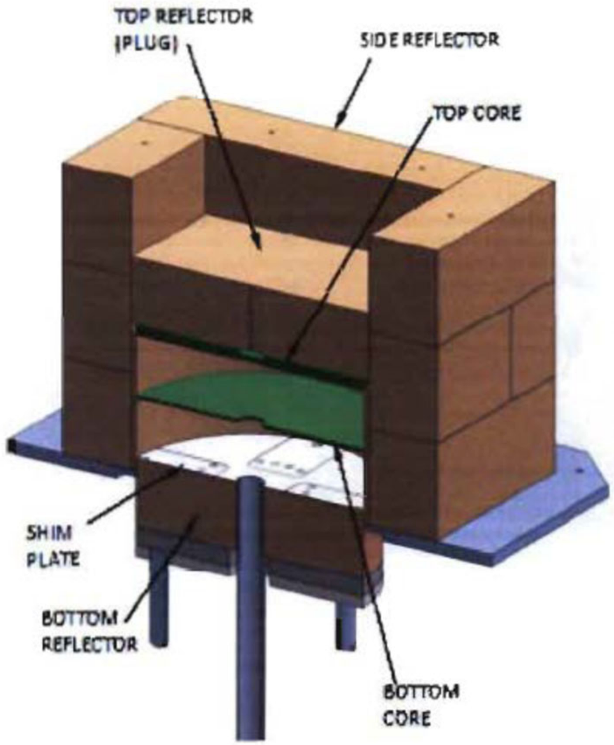


Zeus- General Description

- **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



Preliminary Design: Critical Unresolved Region Integral Experiment

- **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

NCERC
NATIONAL CRITICALITY EXPERIMENTS RESEARCH CENTER

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}U URR Evaluation(s)
  - Assembly reflector/interstitials exist/easily accessible
  - Recent ZEUS measurements performed with Pb →

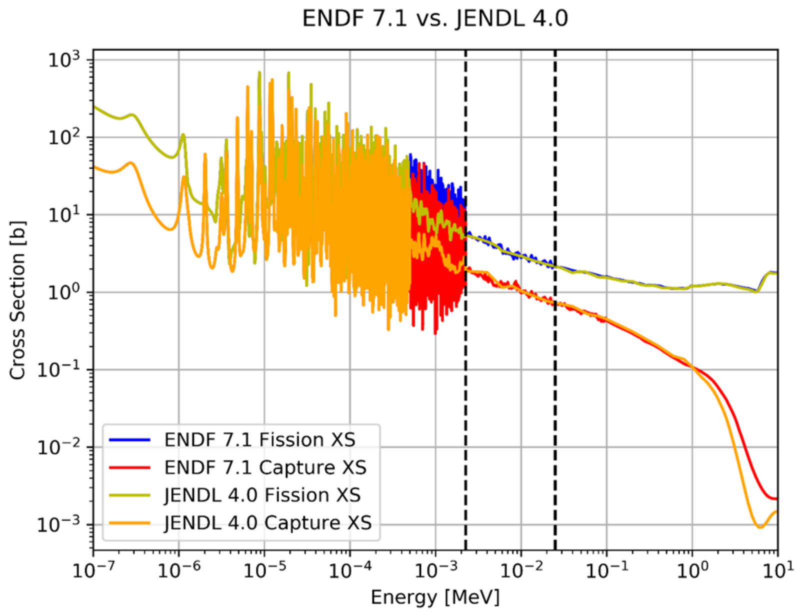
- **Preliminary design of CURIE is the next step**
  - Critical Unresolved Region Integral Experiment (CURIE)
  - Parameters: Reflector/Interstitial/Fuel = Material/Thickness
  - Utilized Physics- Based Approach

- **Final Design**
  - Based on preliminary design, used optimization techniques to down select material

Preliminary Design: Critical Unresolved Region Integral Experiment (CURIE)

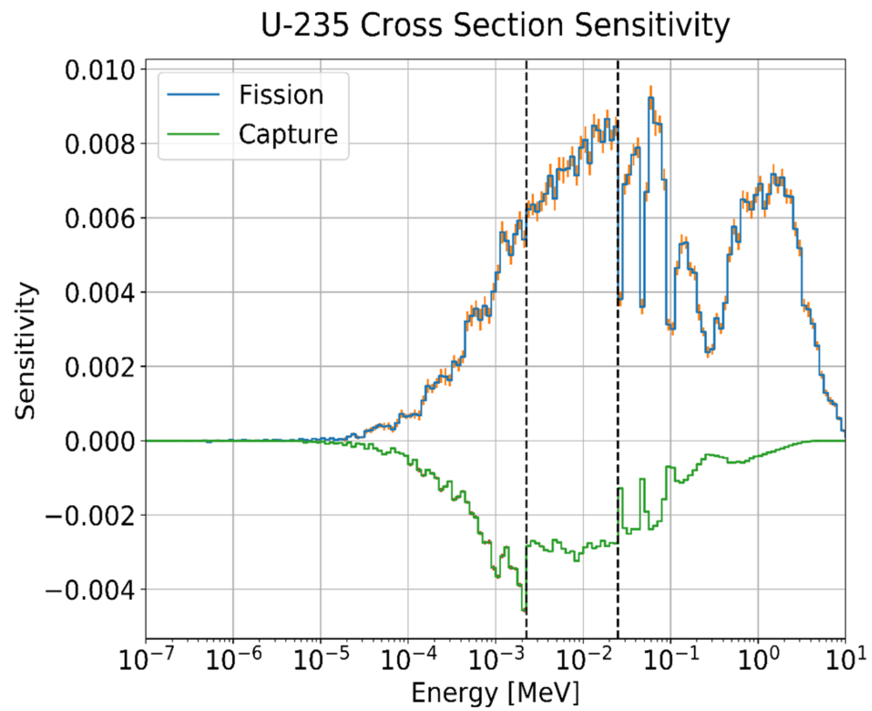
- **URR Region Lacks Validation**
  - Significant variance between data sets

- **Most intermediate energy validation is based on the Zeus series**
  - Current improvements to U-235, Cu-63 and Cu-65 cross sections in the intermediate energy region are based on, and in support of, the Zeus series of benchmarks



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
  - Nuclear Data Quality Associated with Materials



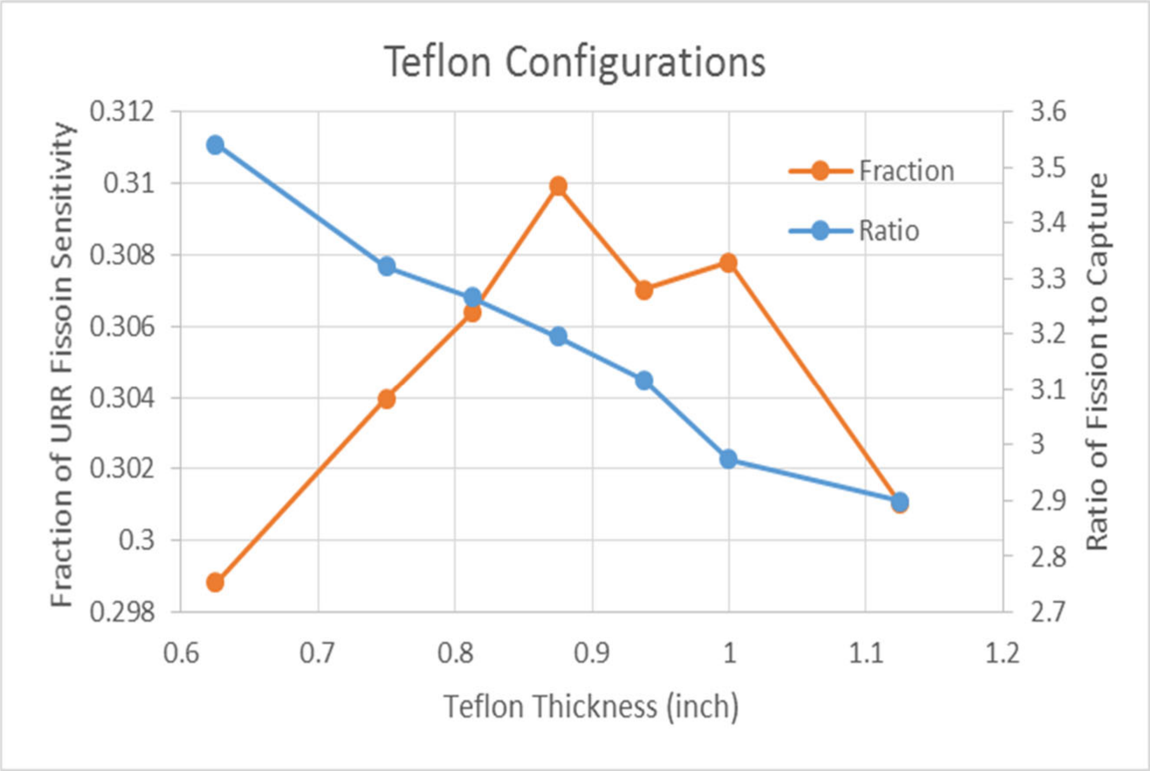
Final Design: Critical Unresolved Region Integral Experiment (CURIE)

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
URR Fission Sensitivity Fraction	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 0.50 to 1.25 inches

Teflon Thickness (inch)	Unit Cells	k_{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



Conclusions and Future Work

Conclusions and Future Work

- CURIE is a needed experiment to support testing of the nuclear data in the URR
- Zeus Series has long history and extensive use in nuclear data improvement efforts

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: ENDF File for URR

Pointed out by Dave Brown for ^{235}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.