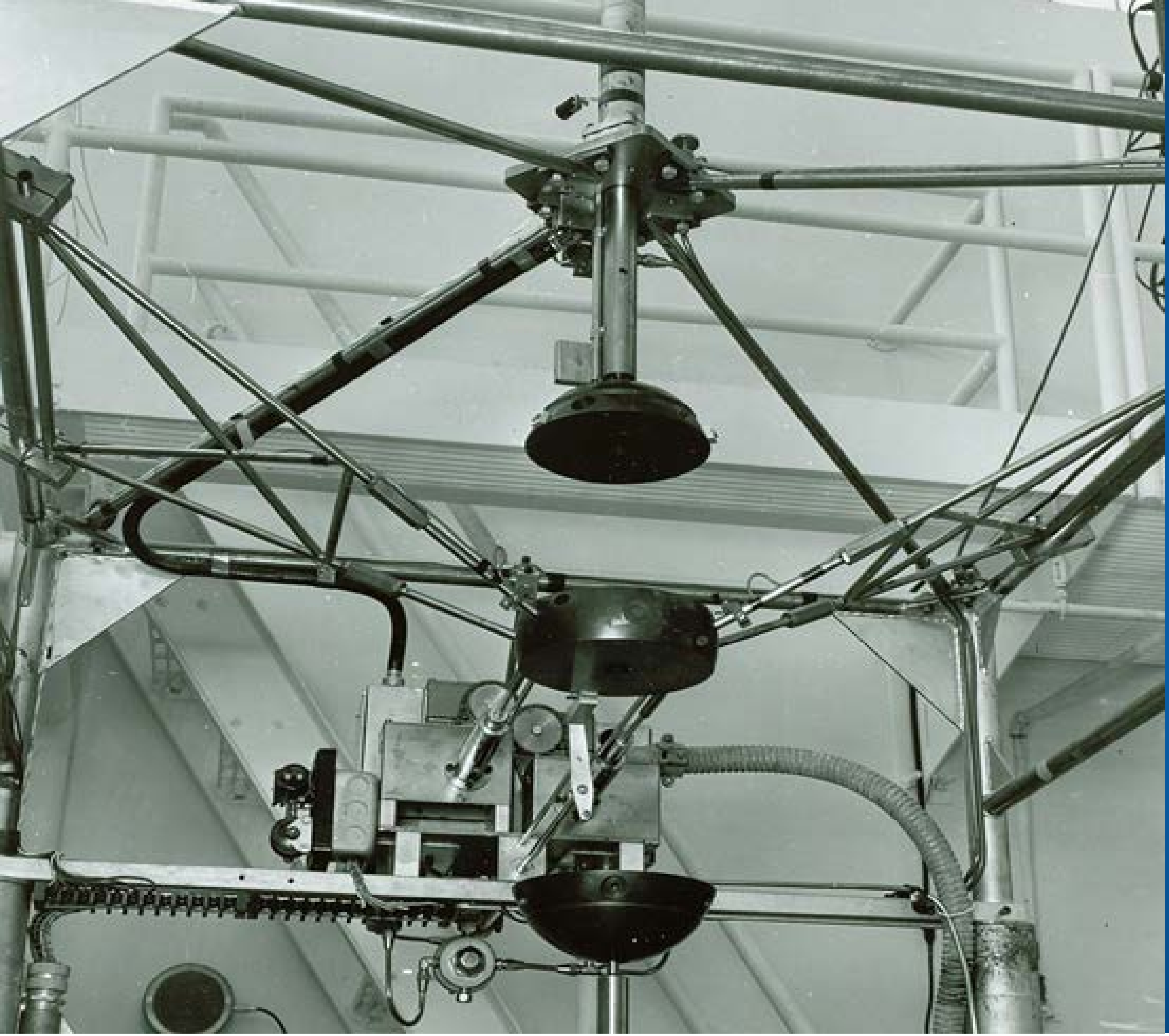

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Delivering science and technology
to protect our nation
and promote world stability

Design of an Intermediate Energy Critical Experiment

for Validation of ^{235}U Unresolved Resonance Region

Nuclear Data and Computational Methods

Rian Bahran

Jesson Hutchinson

Theresa Cutler

Miriam Rathbun

March 2018

NCSP Program Review

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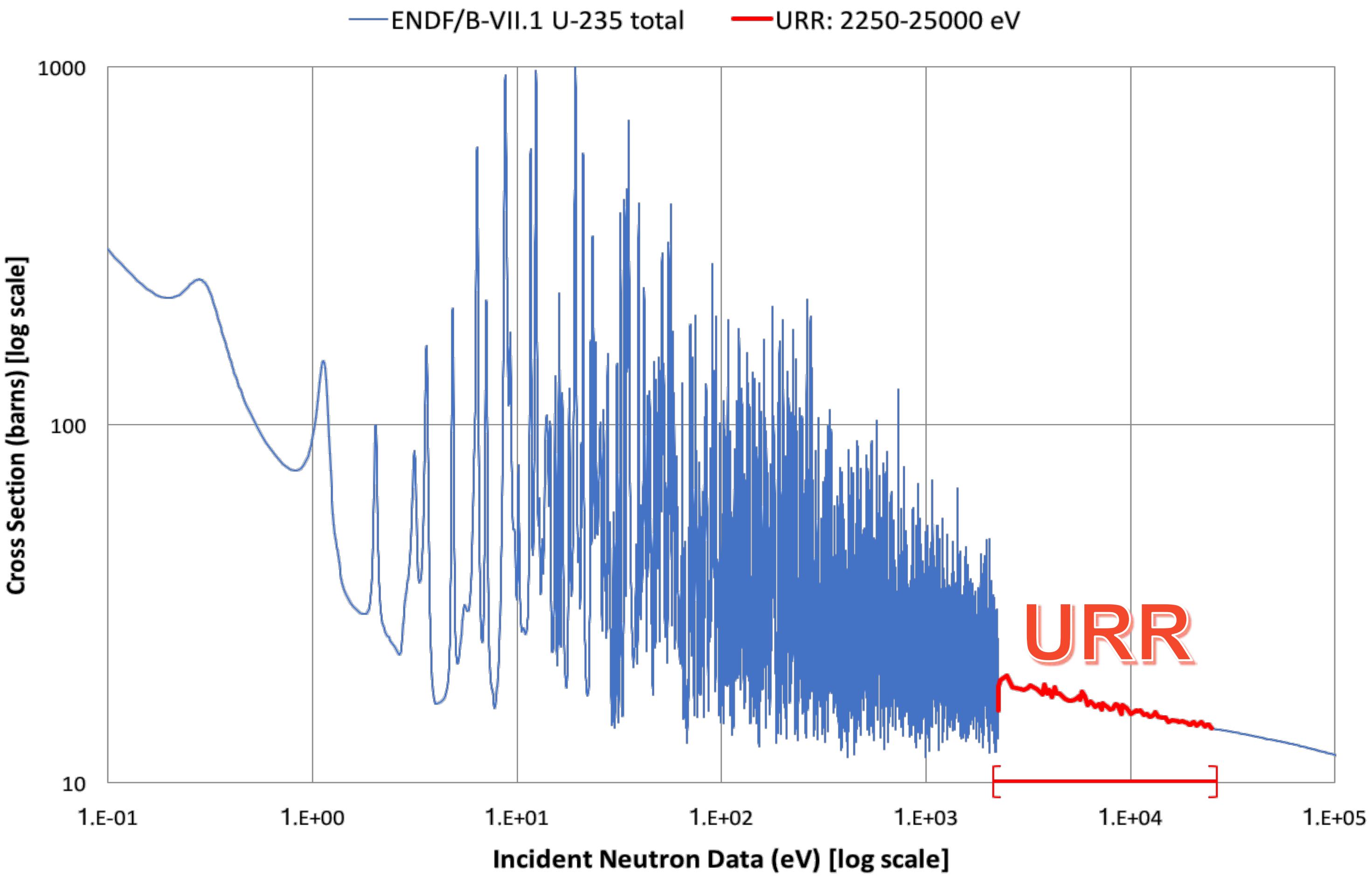
NNSA National Nuclear Security Administration

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

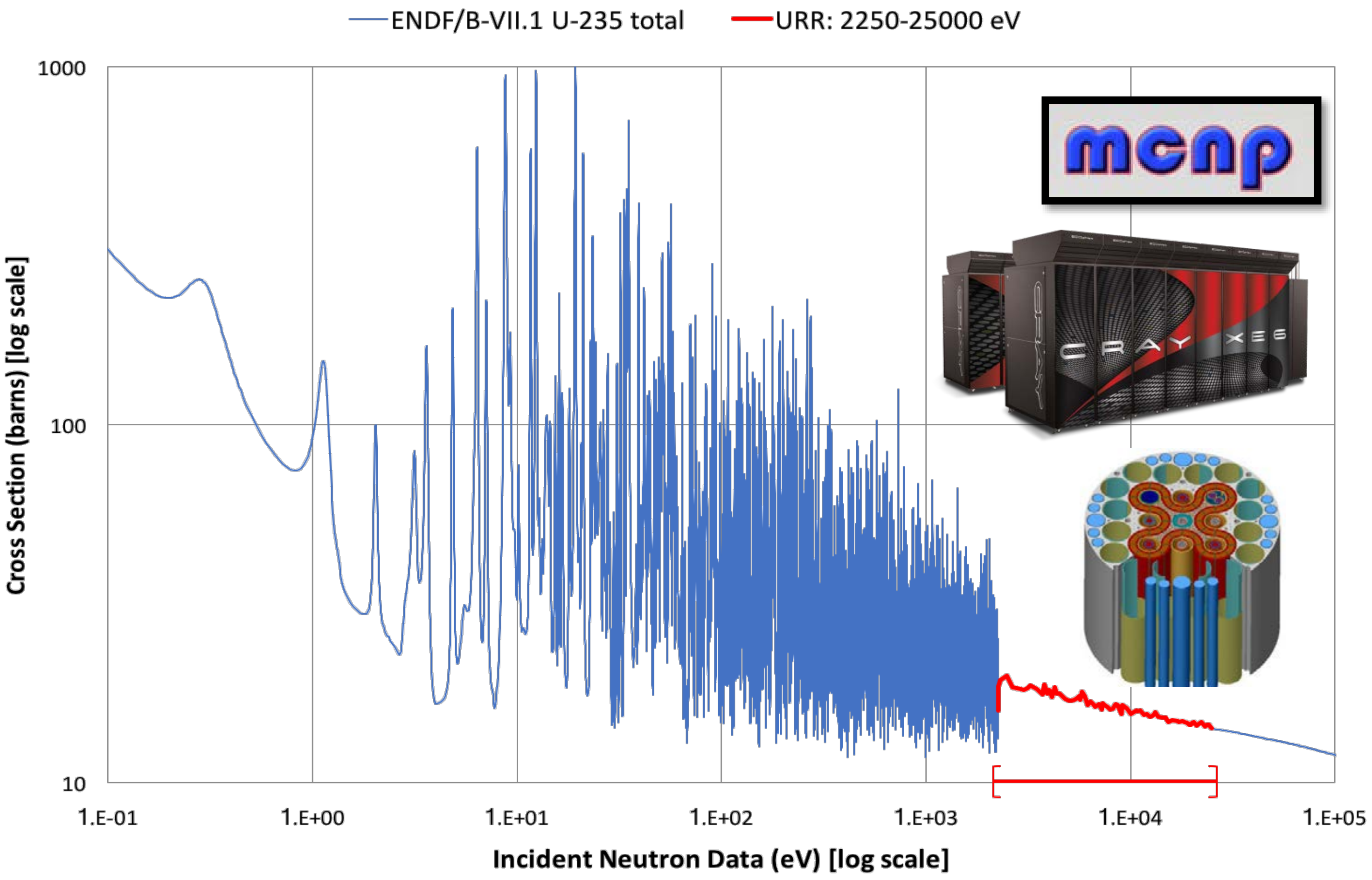
- **The URR is specifically located after the resolved resonance region (RRR) ends, but before the fast (smooth) region begins**
  - There are distinct physical resonances at these energies, but they cannot be fully determined empirically.



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

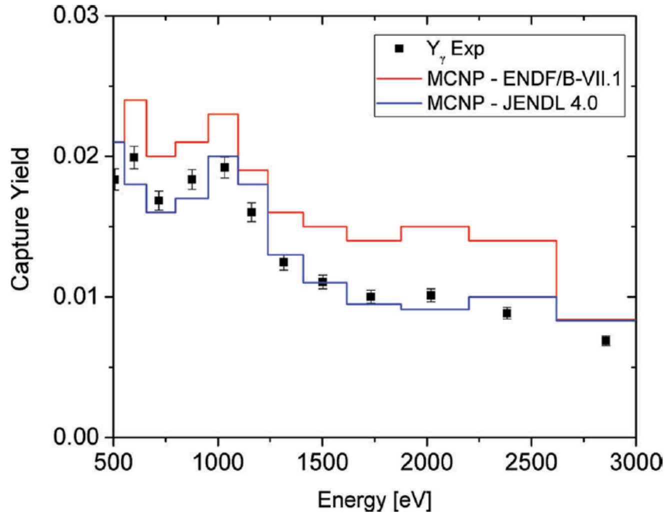


Figure from Y. Danon et al. *Nucl. Sci. and Eng.* (2017)

- **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.

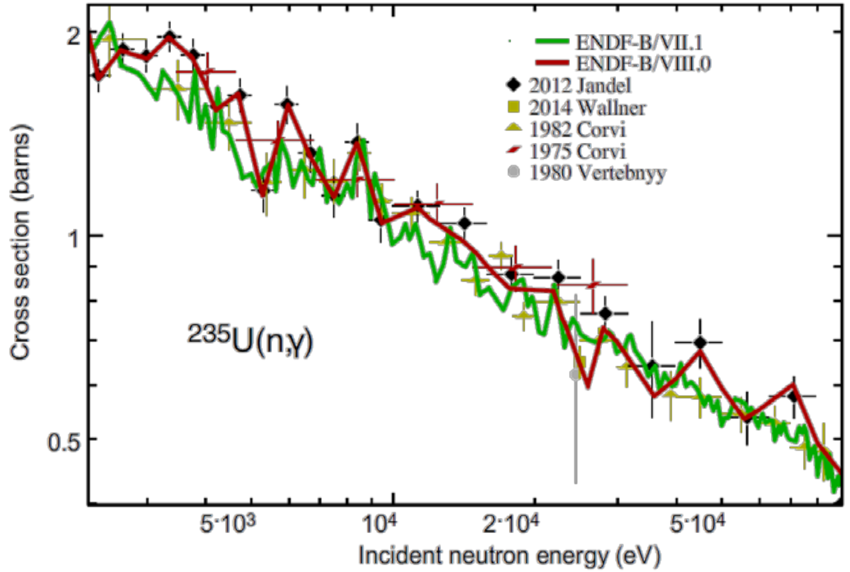


Figure from M. Chadwick et al. *Nucl. Data Sheets* (2018)

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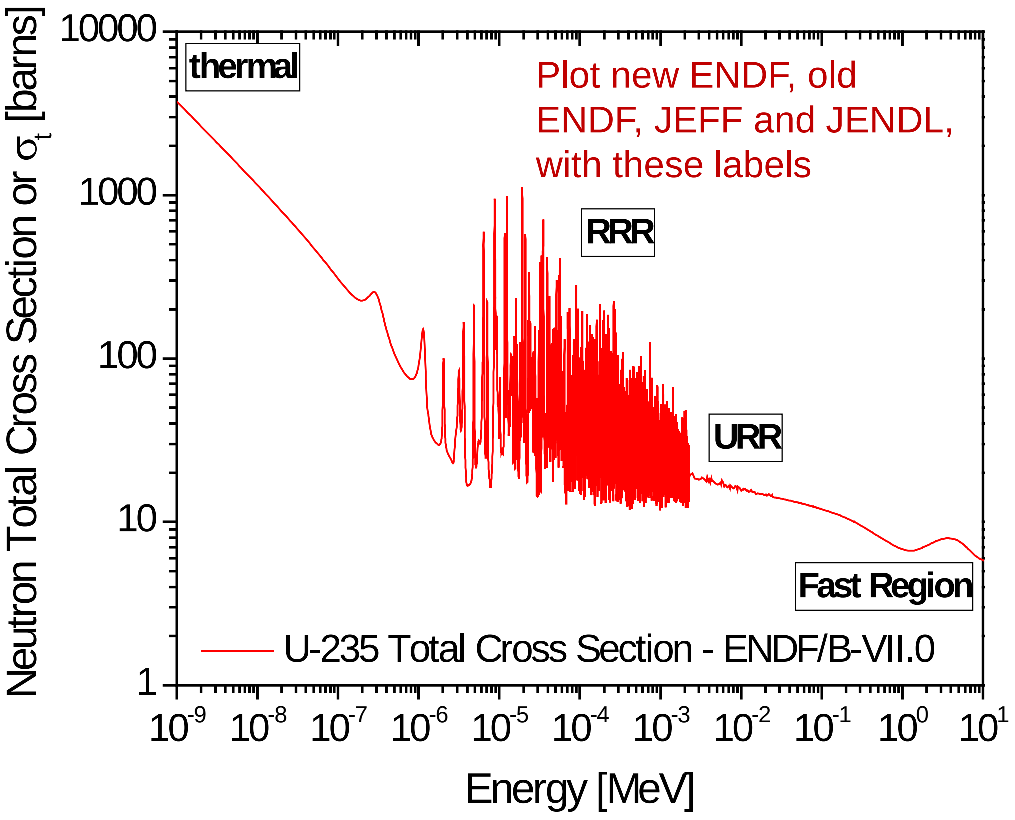
  - New high resolution ^{235}U capture measurements from RPI (Danon et al.) and LANL (Jandel et al.) were significantly below ENDF/B-VII.1 below 2 keV and above it for energies up to 50 keV
- **Recently updated ENDF ^{235}U evaluated file incorporated changes in the URR based on new measurements.**
  - 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.



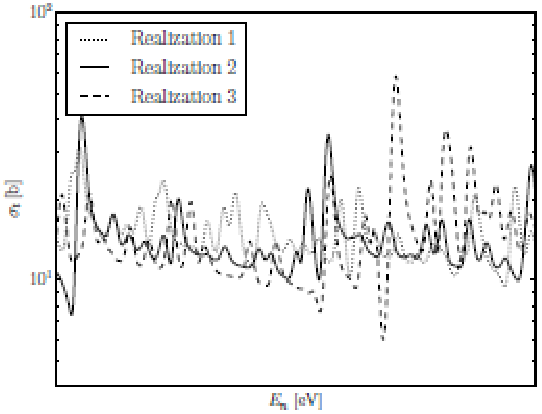
^{235}U URR Bounds for Several Data Libraries

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

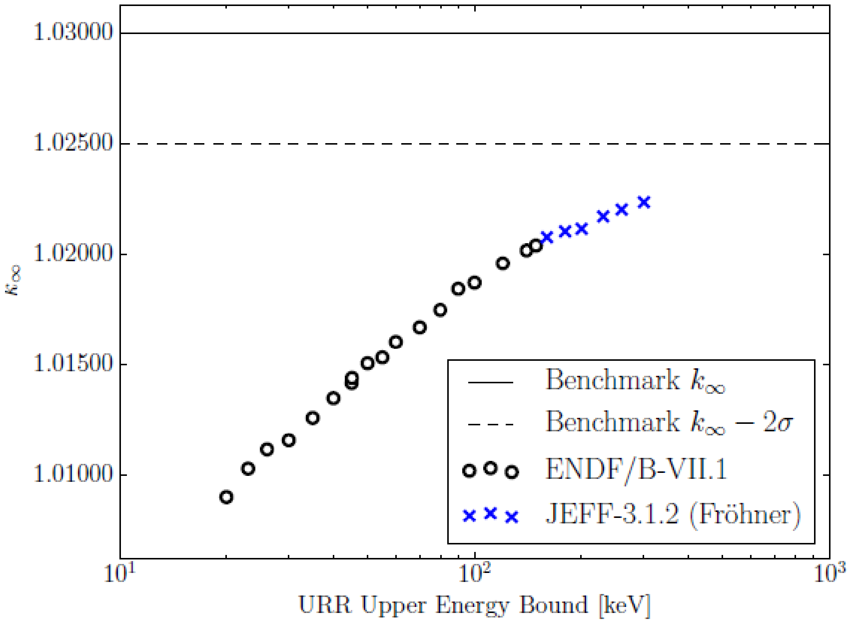
Why is the Unresolved Resonance Region for 235U important to re-visit?

#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.



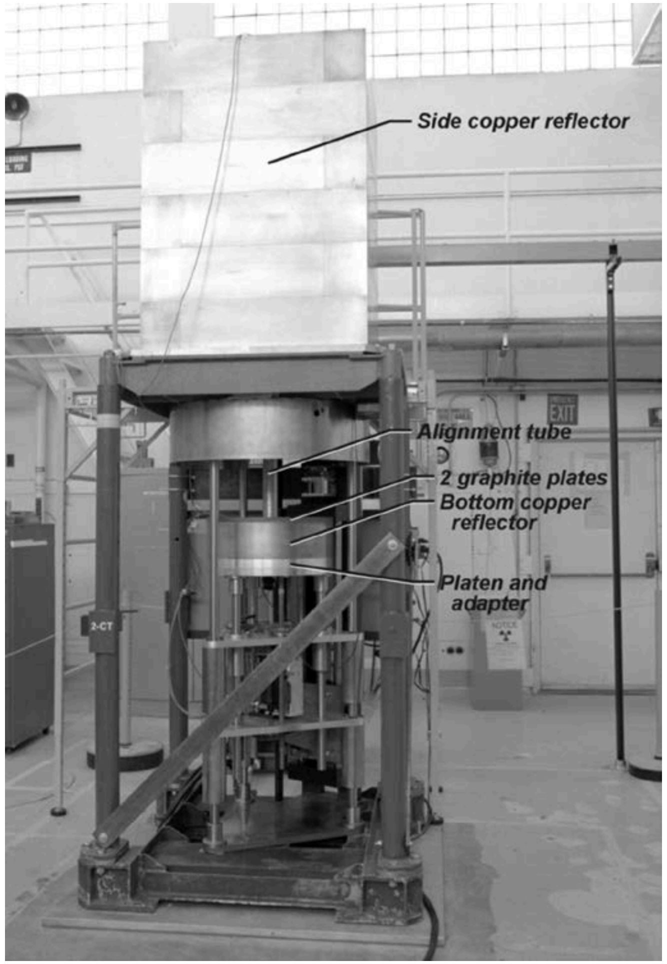
OpenMC



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.



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.

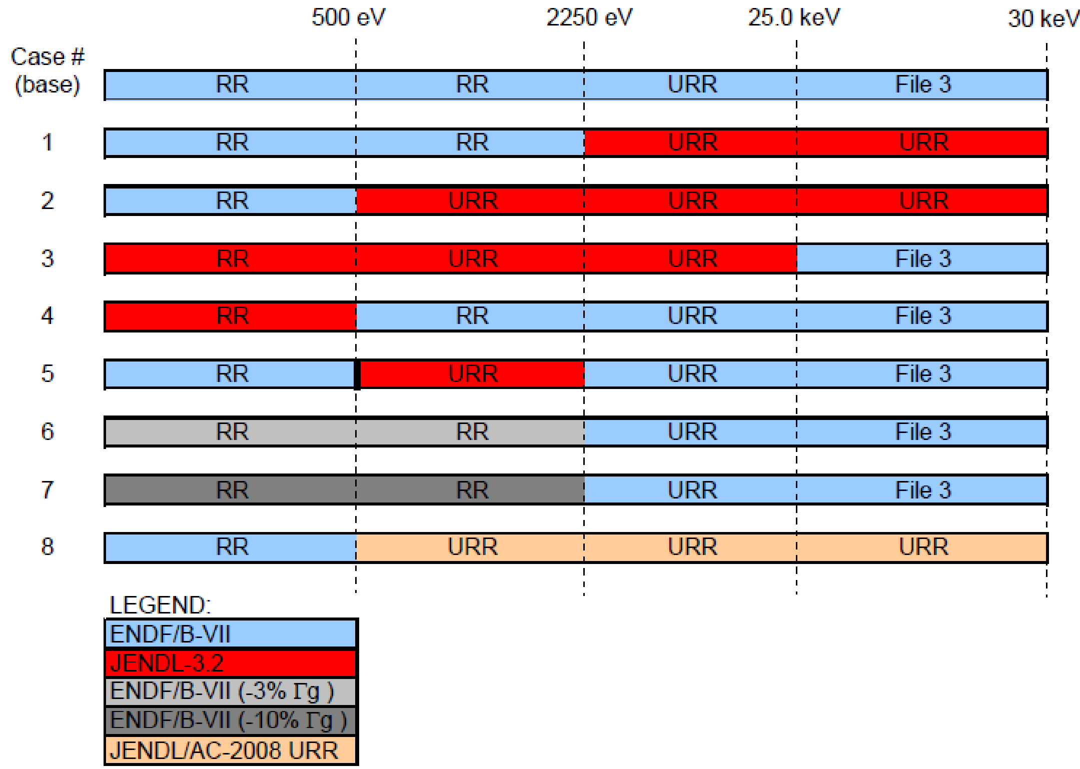
Benchmark	Experimental k_{eff}	MCNP ENDF66	MCNP ENDF66 with ^{235}U ORNL Evaluation
ORNL10	1.0015 ± 0.0010	0.9987 ± 0.0004	0.9991 ± 0.0004
HISS/HUG	1.0000 ± 0.0040	1.0099 ± 0.0005	1.0092 ± 0.0005
UH_3 (1)	1.0000 ± 0.0047	1.0040 ± 0.0050	1.0020 ± 0.0005
Zeus (1)	0.9976 ± 0.0008	0.9918 ± 0.0003	0.9899 ± 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

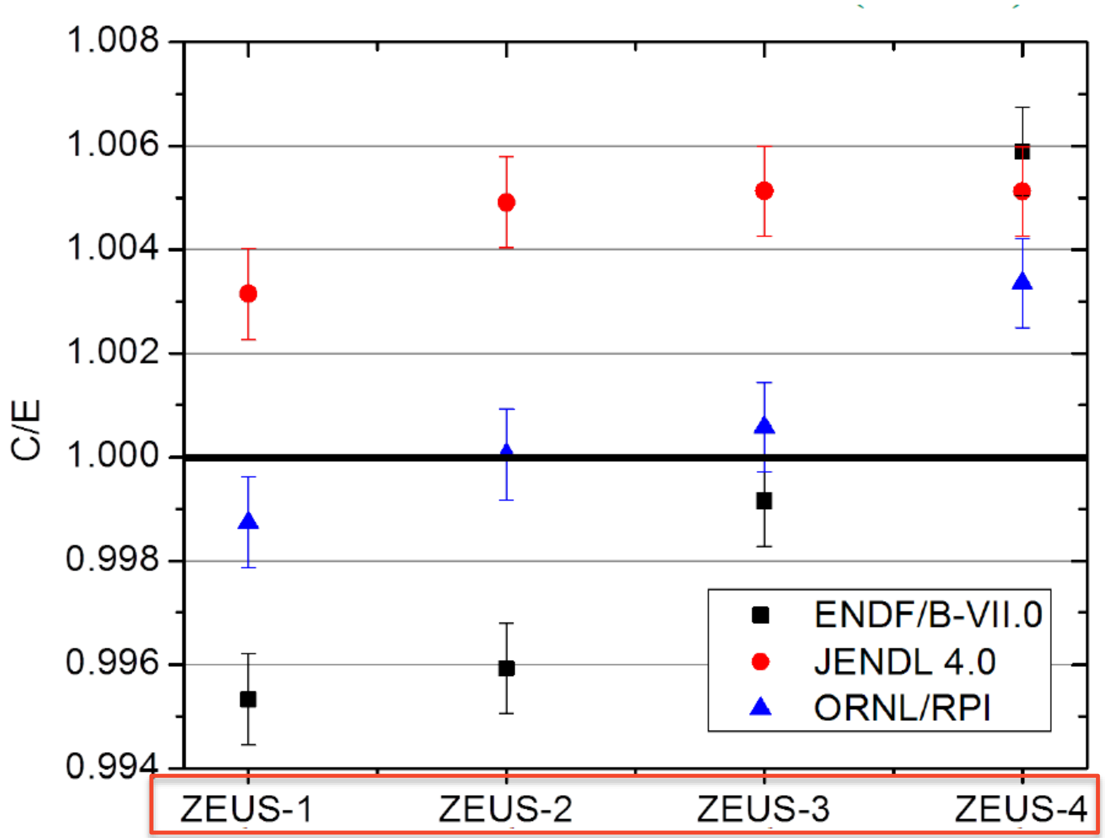
Table 2. Energy of the average lethargy causing fission (AVG)

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.

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- **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.
- **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

Experiment Preliminary Design

Neutrons are Born Fast and are Easy to Thermalize…

- **Which makes the design and execution of intermediate neutron energy experiments a challenge!**
  – Integral measurements require very large moderated/reflected systems.

ZEUS (LANL) and ZEBRA-8H (UKAEA)
integral measurements

Neutrons are Born Fast and are Easy to Thermalize…

- **Which makes the design and execution of intermediate neutron energy experiments a challenge!**
  - – Integral measurements require very large moderated/reflected systems.
  - – Differential measurements may require long measurement times….

ZEUS (LANL) and ZEBRA-8H (UKAEA)
integral measurements

RPI Linear Accelerator
differential measurements

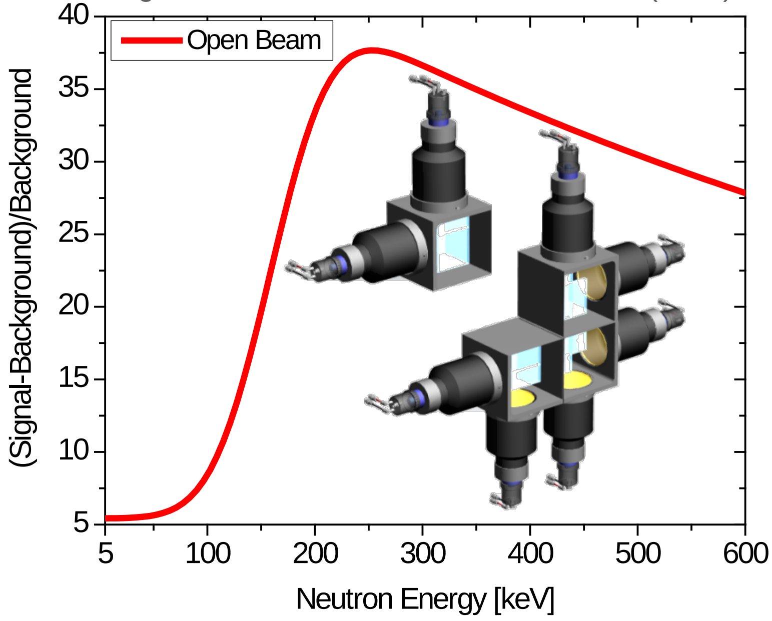
Neutrons are Born Fast and are Easy to Thermalize…

- **Which makes the design and execution of intermediate neutron energy experiments a challenge!**
  - Integral measurements require very large moderated/reflected systems.
  - Differential measurements may require long measurement times… and can suffer from high background rates.

ZEUS (LANL) and ZEBRA-8H (UKAEA)
<u>integral measurements</u>

RPI Linear Accelerator
<u>differential measurements</u>

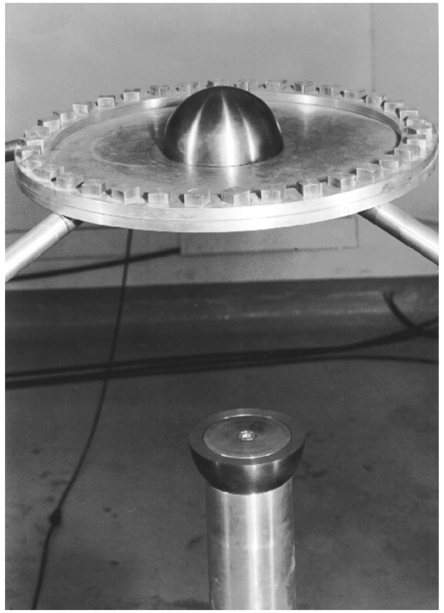
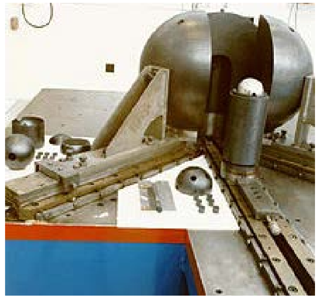
Figure from R. Bahran, *PhD Dissertation* (2013)



One of Several RPI Intermediate Energy Neutron Detector
<u>differential measurements</u>

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

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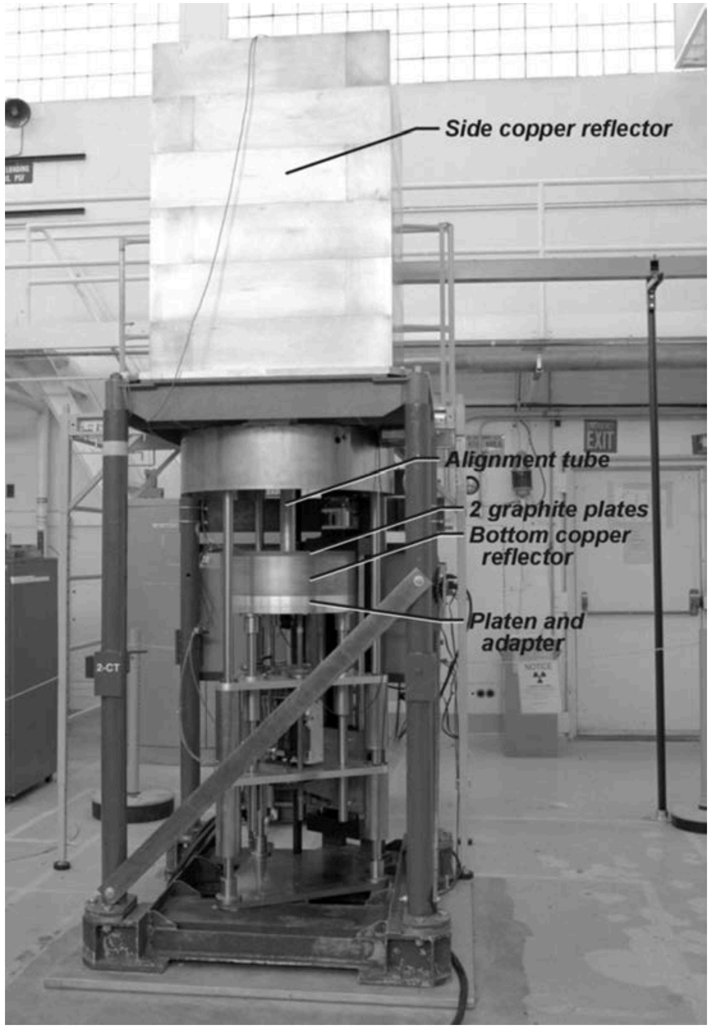
  - Used in most recent ^{235}U URR Evaluation(s)



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- **ZEUS is a good starting point**
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  - Assembly reflector/interstitials exist/easily accessible
  - Recent ZEUS measurements performed with Pb

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

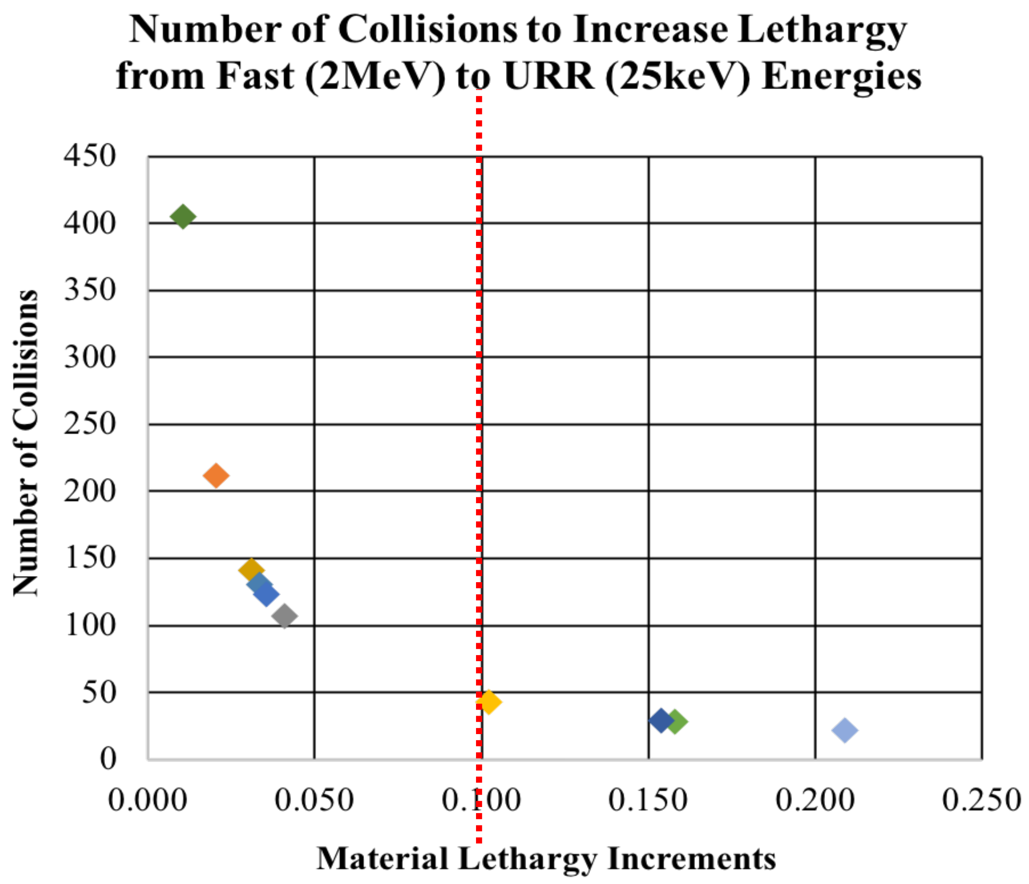
- **ZEUS is a good starting point**
  - Used in most recent ^{235}U URR Evaluation(s)
  - Assembly reflector/interstitials exist/easily accessible
  - Recent ZEUS measurements performed with Pb →

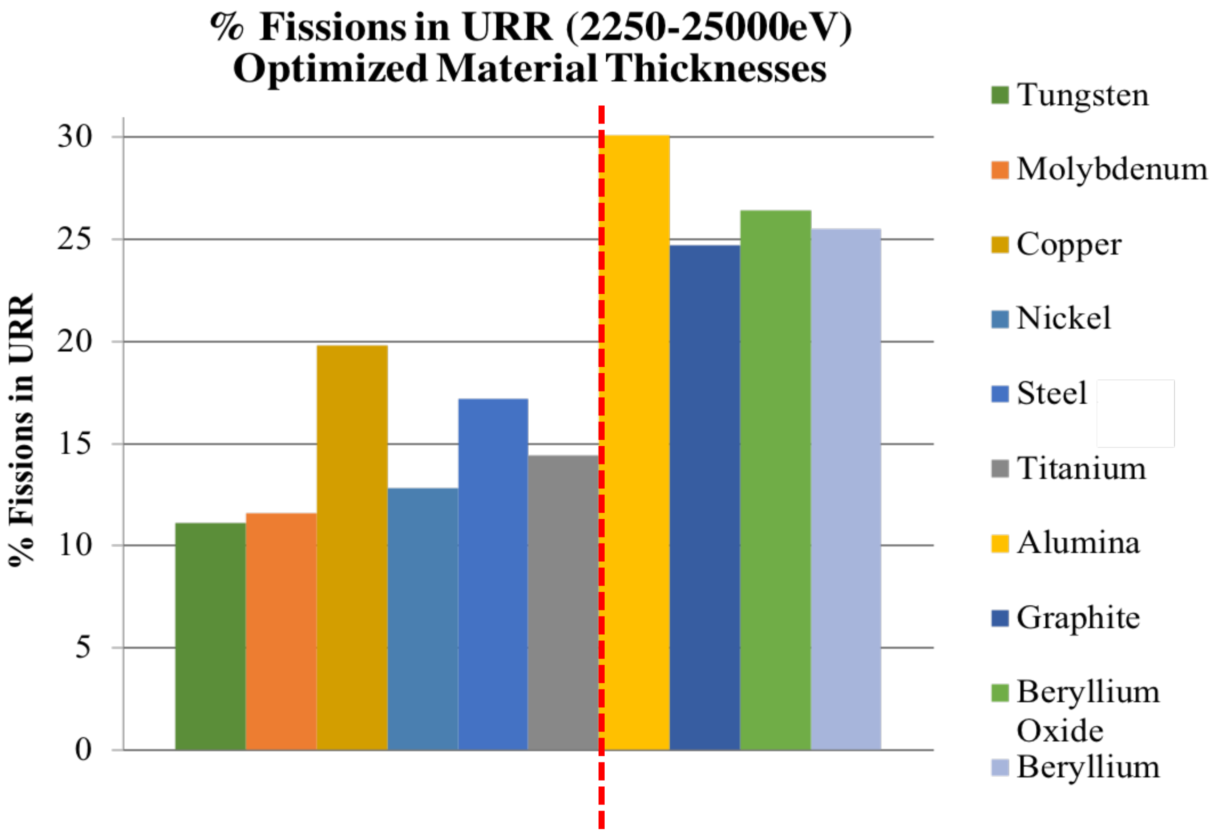
- **Preliminary design of CURIE is the next step**
  - Critical Unresolved Region Integral Experiment (CURIE)
  - Parameters: Reflector/Interstitial/Fuel = Material/Thickness
  - Physics-Based Material Selection (Analytical + Monte Carlo)
    - Energy Loss Per Collision
    - Mean Free Path
    - Competing Reactions

CURIE Physics-based materials selection: Energy Loss per collision

Use average lethargy increments to determine moderating power.

Success criteria: $\zeta > 0.1$

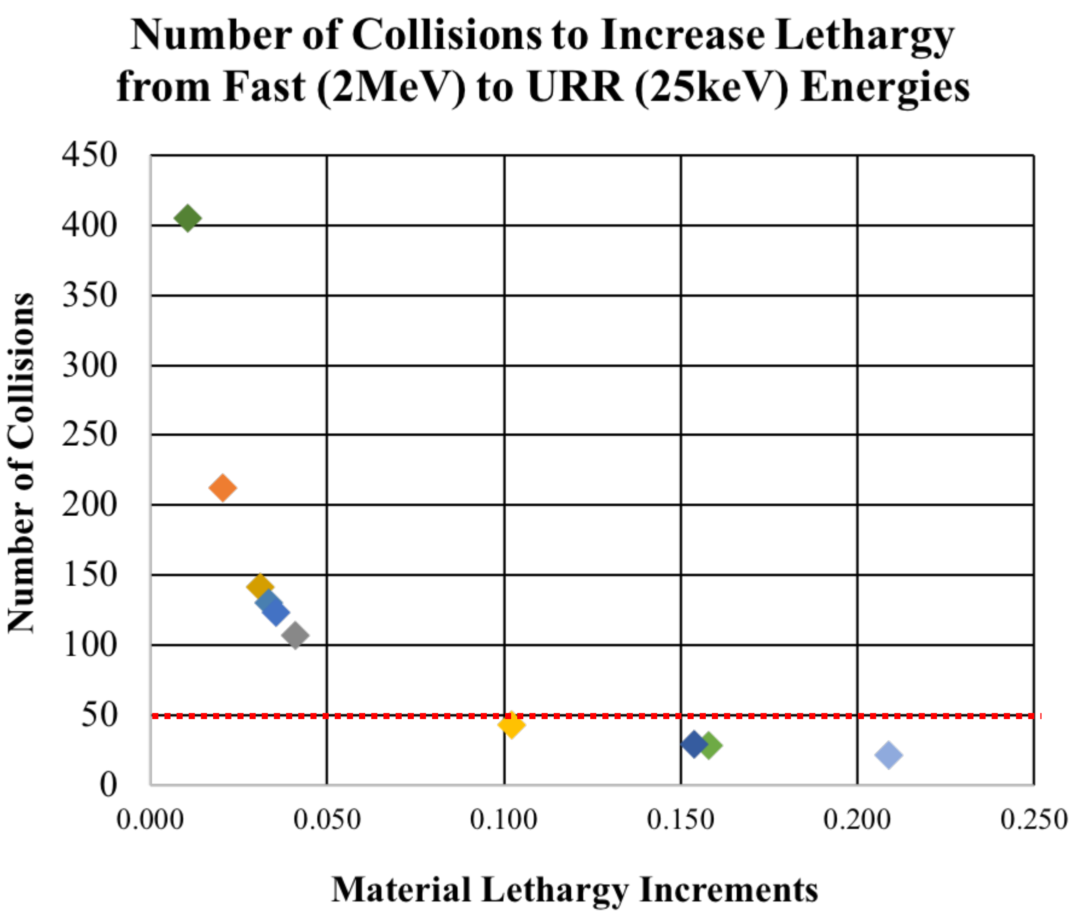


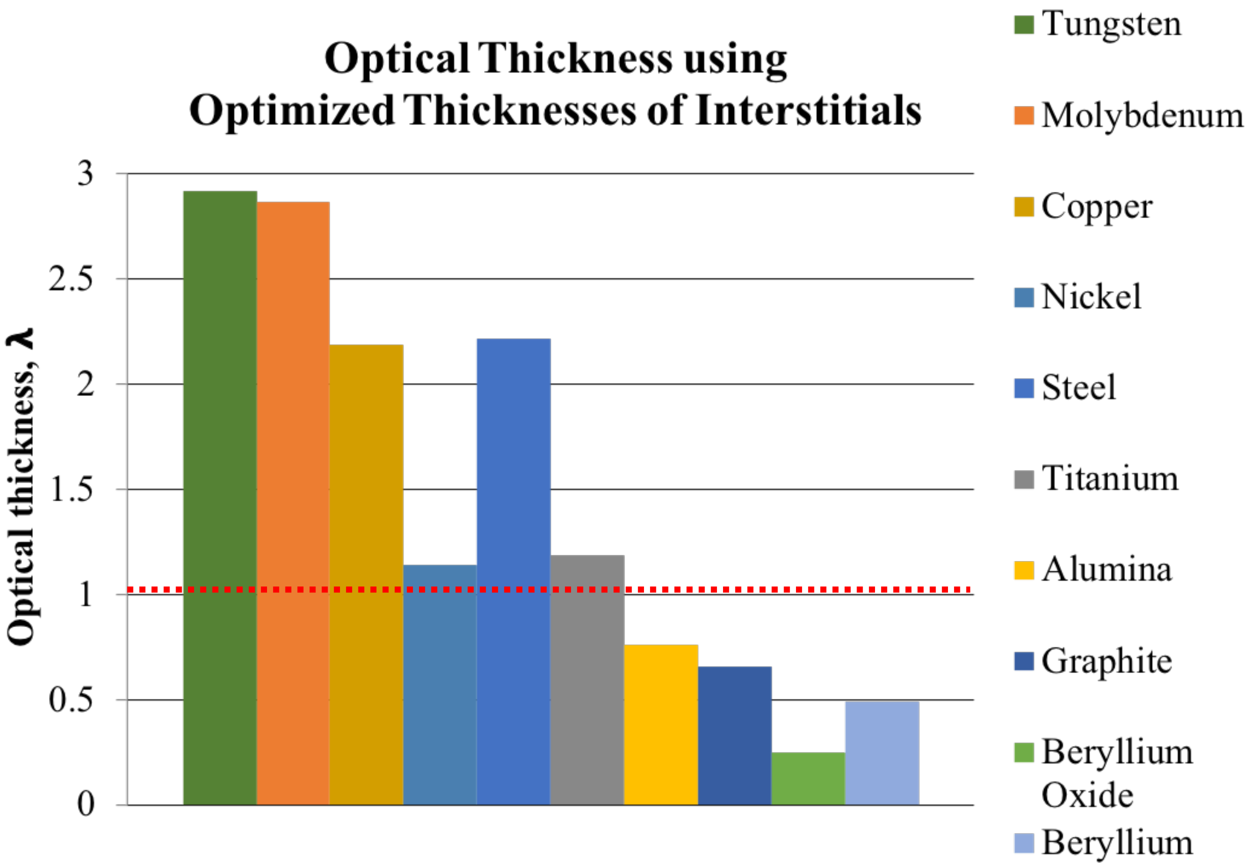


CURIE Physics-based materials selection: Optical thickness

Optical thickness: $\lambda = \frac{t\ [cm]}{MFP\ [cm]}$

Success criteria: $\lambda < 1$

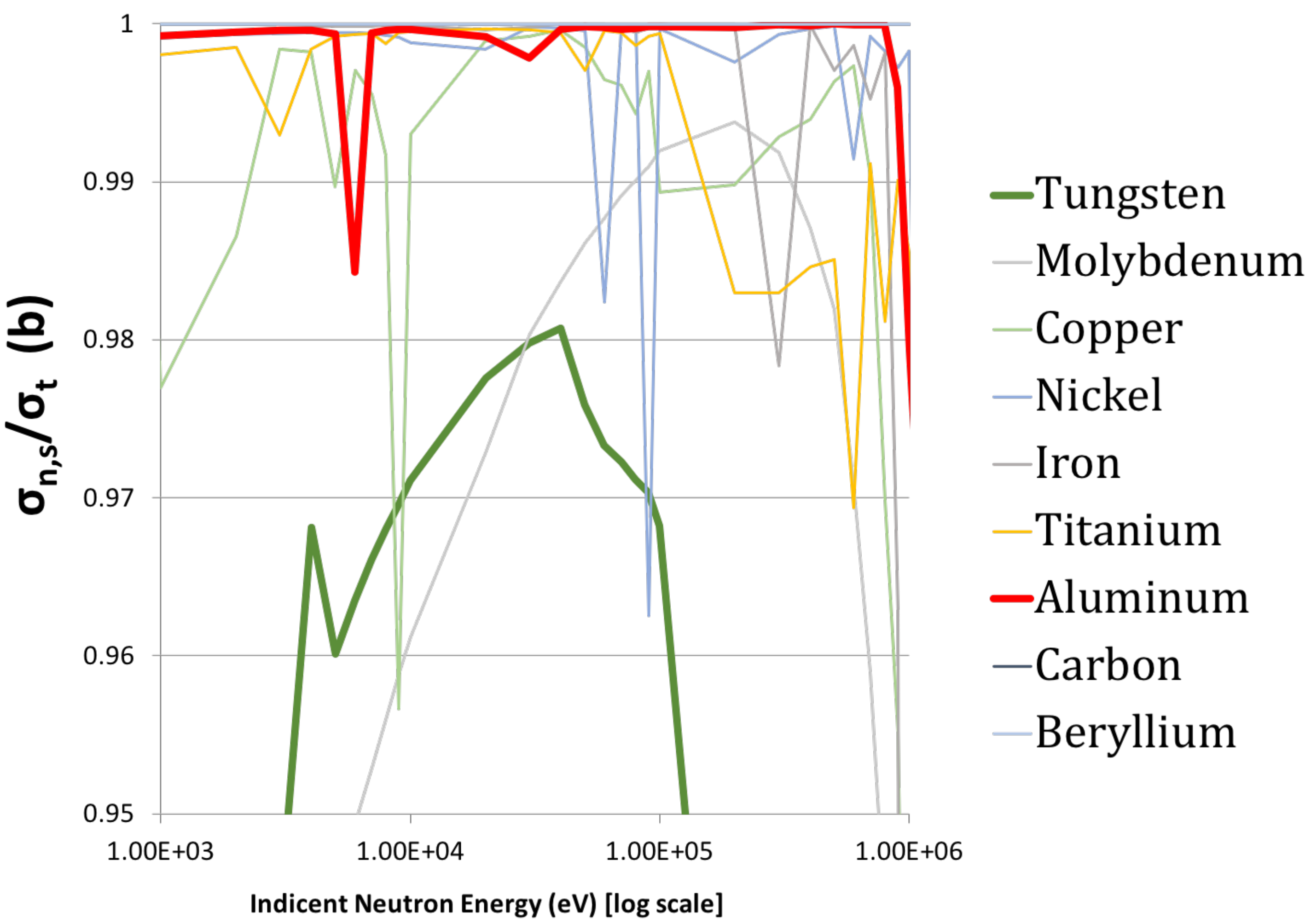




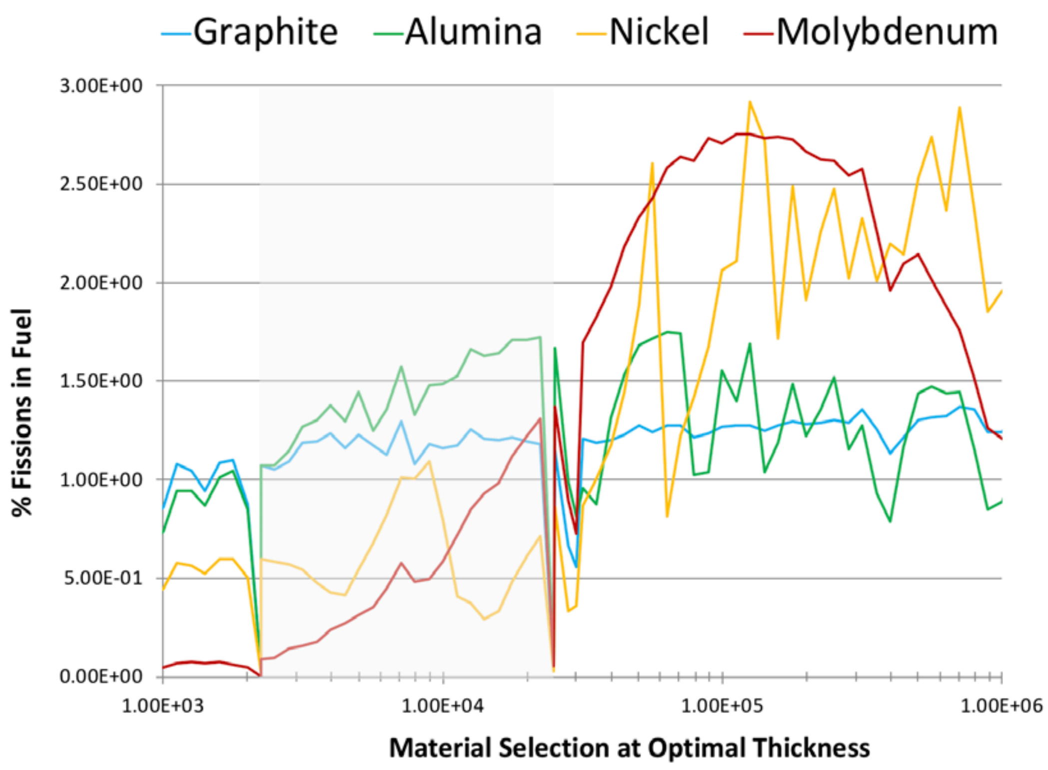
CURIE Physics-based materials selection: Competing reactions

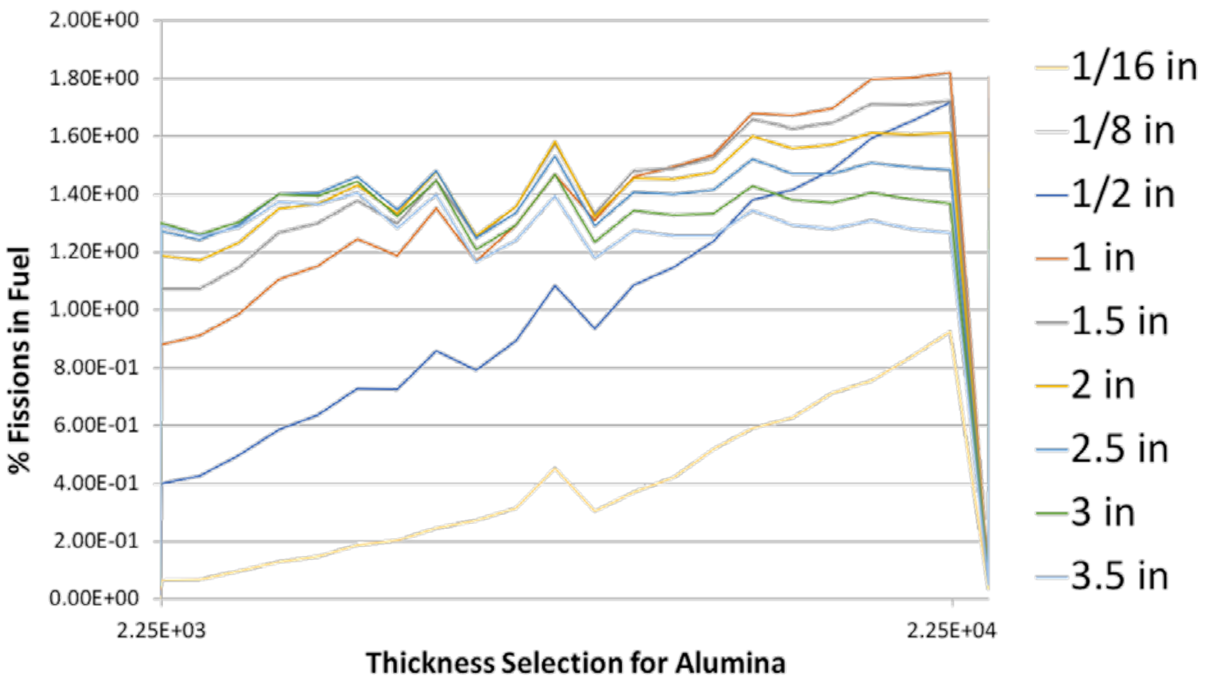
- **Avoid competing reactions from your moderator and reflector.**
  - Compare scatter to total cross section.
  - Competing reactions will preferentially "not scatter neutrons" towards the URR.
  - Competing reactions will also preferentially absorb URR neutrons once they are in the right energy range.
  - Competing "resonance reactions" might add unwanted uncertainty in predictive simulations, since this is a difficult differential regime for measuring high resolution structure.

- **Qualitative assessment on "competition"**
  - Assessment should span energies from URR onwards.



CURIE Physics-based materials selection: Optimizing Thickness

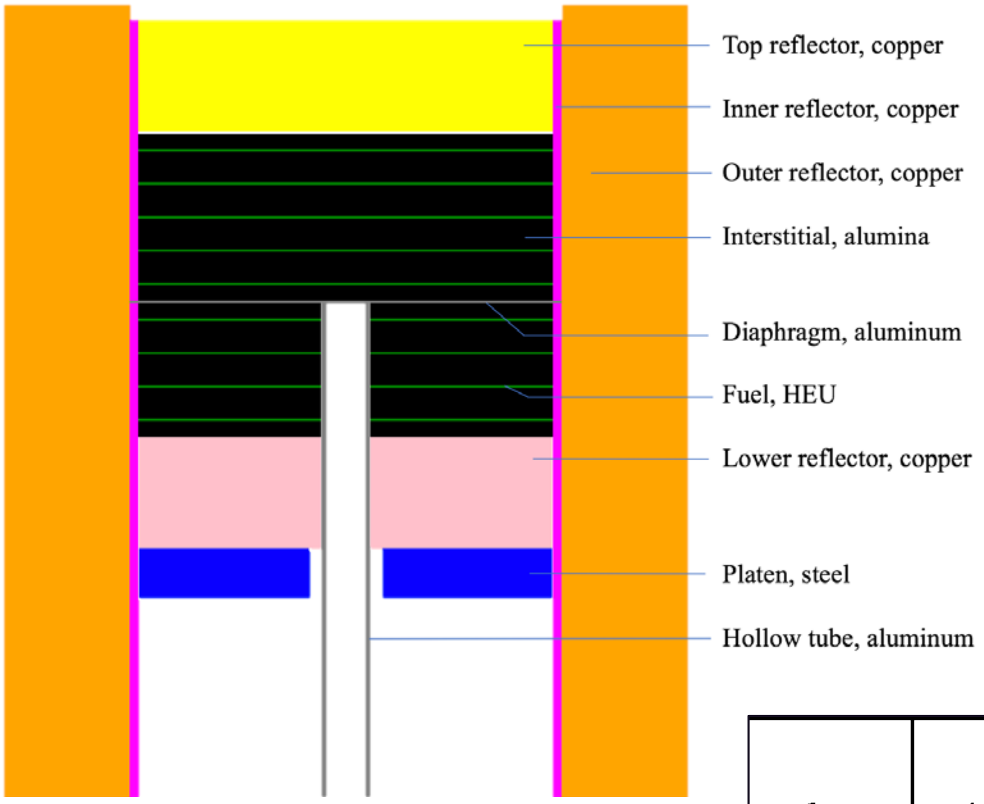




CURIE Physics-based Materials selection: Summary

	Lethargy	MFP (cm)	t (cm)	λ	Competing Reaction Test	% Fissions in URR (Results)
Common Success Criteria	> 0.1			< 1	✓	
Beryllium	**0.209**	2.19	1.3	**0.49**	✓	**25.5**
Beryllium Oxide	**0.154**	2.12	1.3	**0.25**	✓	**26**
Graphite	**0.158**	5.01	3.8	**0.66**	✓	**24.5**
Alumina	**0.1**	3.23	3.8	**0.76**	✓	**31**
Titanium	0.041	4.44	6.35	1.19		14
Steel	0.036	3.33	8.9	2.22		17
Nickel	0.034	2.71	3.8	1.14		12.5
Copper	0,031	3.34	8.9	2.19		19.5
Molybdenum	0.021	2.36	8.9	2.87	x	12
Tungsten	0.011	1.81	7.6	2.92	x	11

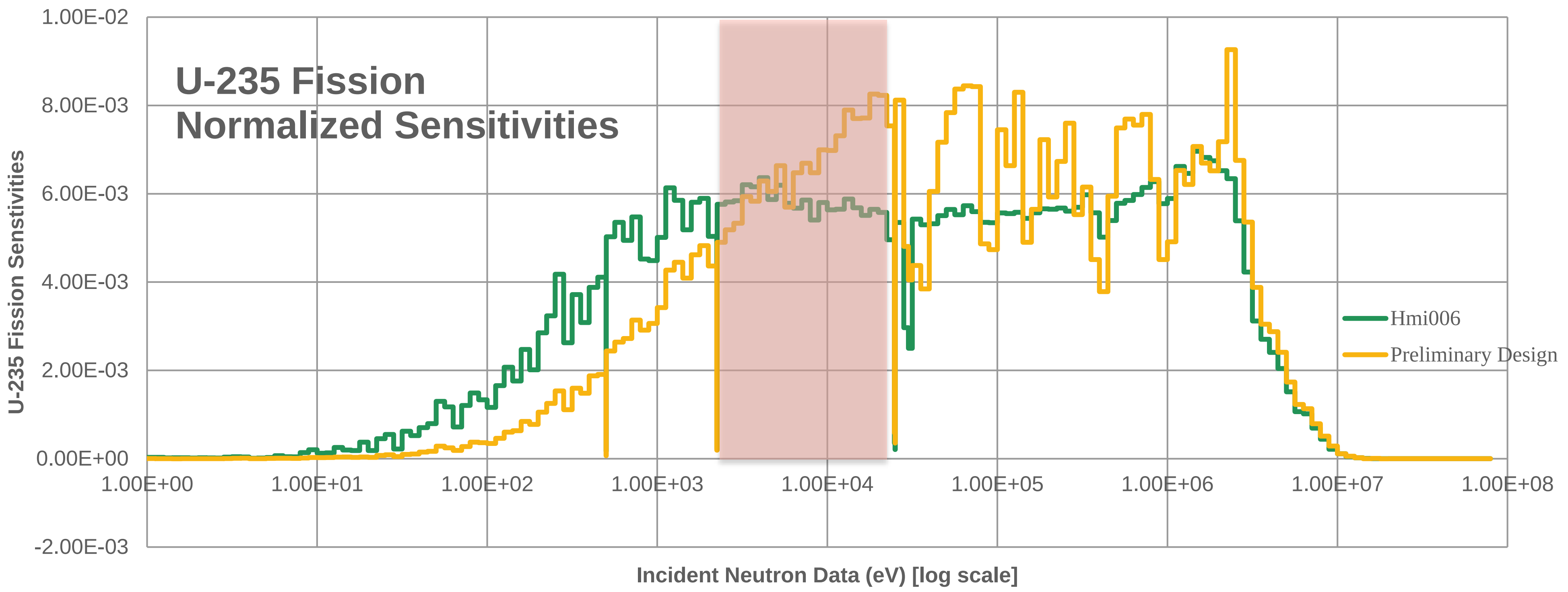
CURIE Preliminary Design: Results



- **CURIE Preliminary Design**
  - Alumina interstitial: 1.5 inch
  - HEU fuel: 9 plates, 0.118 inch
  - Copper Reflector
  - Flux and Fission profiles (below) based on ENDF/B-VII.I
- **Need comparison to past ZEUS Benchmarks**
  - HEU-MET-INTER-006 i.e. HEU w/graphite intersitial
  - Most sensitive existing intermediate benchmark
  - Used as basis for all recent 235U intermediate energy evaluations.

k_{eff}	AFGE	% Flux			% Fission Neutrons		
		Thermal <0.7 eV	Intermediate 0.7 eV-100 keV	Fast >100 keV	Thermal <0.7 eV	Intermediate 0.7 eV-100 keV	Fast >100 keV
0.98487	3.92E+05	2.76E-05	44.43	55.57	1.12E-03	66.01	33.99
		URR (2.25 keV-25 keV): **20.37**			URR (2.25 keV-25 keV): **31.07**		

CURIE Preliminary design: Comparison to ZEUS



	CURIE	Hmi006
Percent Overall Sensitivity in the URR	0.528%	0.465%
Δk_{eff} with URR modules	0.064%	0.035%
% Fissions in Intermediate Range 0.7 eV-100 keV	66.79%	63%
% Fissions in URR 2.25 keV-25 keV	**31.07%**	**27%**

Conclusions and Future Work

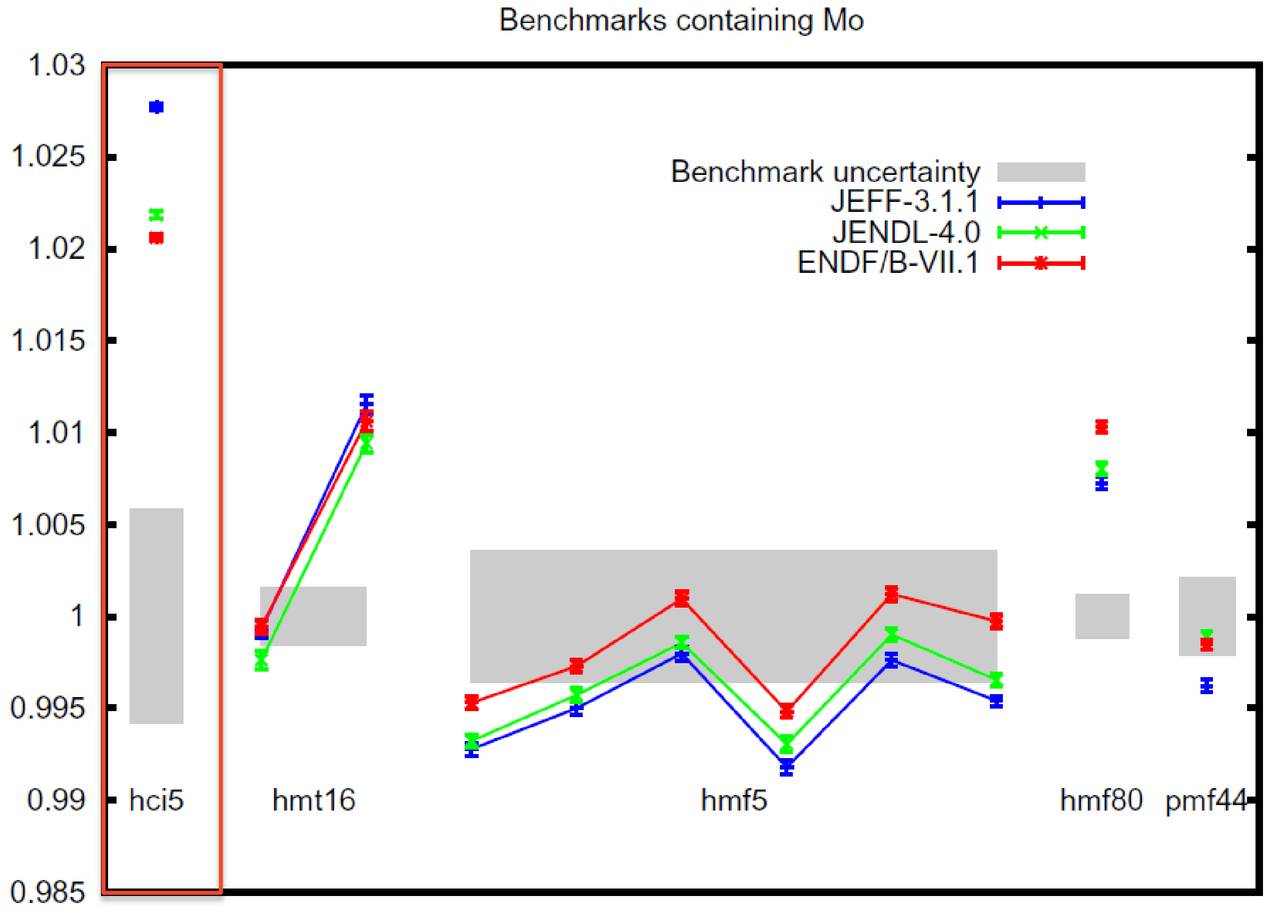
Conclusions and Future Work

- **Assess CURIE preliminary design against additional libraries**
  - newest ENDF, JEFF, and JENDL
- **Evaluate specific contributions to keff from other parameters beyond fission**
  - Capture cross section
  - Average parameter values and URR boundaries
- **Explore sensitivities to ^{238}U Subject to similar updates in evaluation.**
- **Explore similar designs for other intermediate energy nuclear data needs**
  - ^{238}U (CURIE might suffice)
  - Re-visiting Molybdenum (needs new intermediate integral experiment)

Re-visiting Molybdenum Intermediate Energy Data

- **Integral Benchmarks**
  - Sparse - only one (discrepant) HEU-inter, no Pu-inter
  - Discrepancy - several thousand pcm difference

Figure from S. C. Mark *Nuclear Data Sheets* (2012)



Re-visiting Molybdenum Intermediate Energy Data

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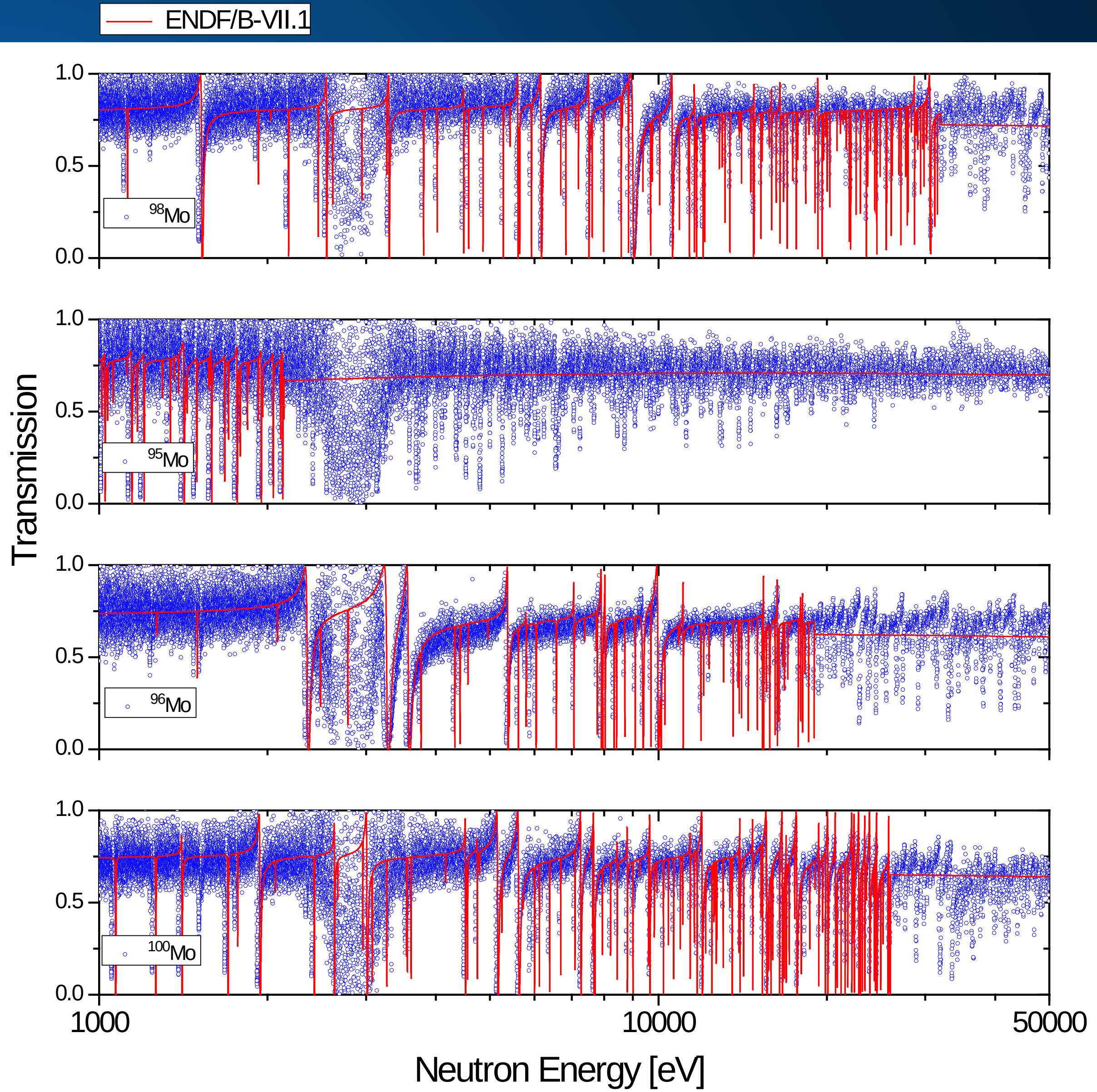
- **Differential Data**
  - Disagreements between international evaluations including average parameters and upper URR boundaries
  - Recent RPI (Danon) high resolution isotopic Mo intermediate energy data

Figure from R. Bahran, Y. Danon et al. *Phys Rev C.* (2013)



Re-visiting Molybdenum Intermediate Energy Data

- **Integral Benchmarks**
  - Sparse - only one (discrepant) HEU-inter, no Pu-inter
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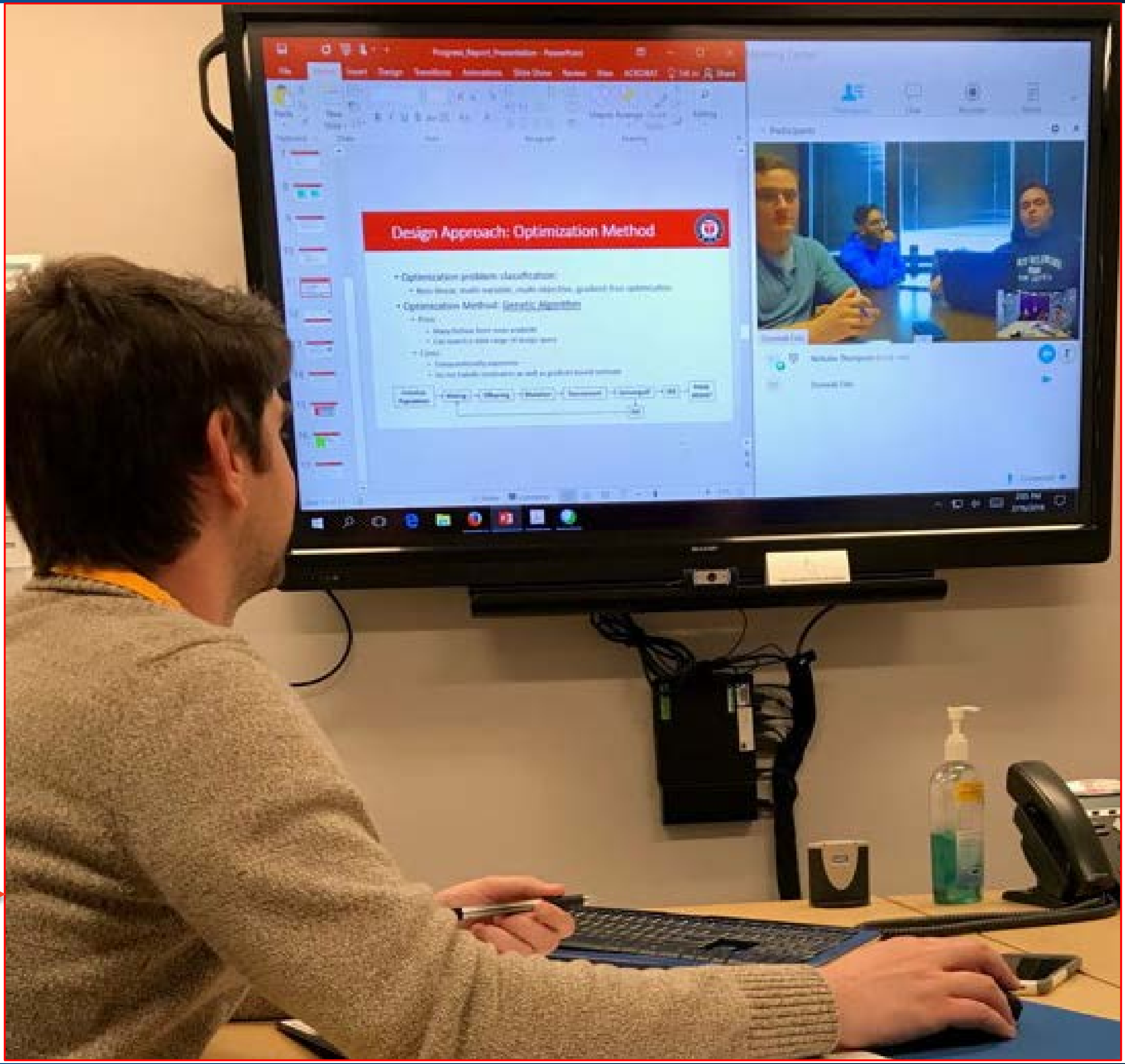
- **Differential Data**
  - Disagreements between international evaluations including average parameters and upper URR boundaries
  - Recent RPI (Danon) high resolution isotopic Mo intermediate energy data
- **RPI Nuclear Engineering Senior Design Capstone Project Team**
  - Exploring the design of a Mo-based intermediate benchmark.
  - Applying Machine-Learning to exploring the design space.
  - Working <u>remotely</u> with LANL Critical Experiments Team: J. Hutchinson, T. Cutler, R. Bahran, N. Thompson
  - One of the team members (Dominik Fritz) will be joining LANL in the summer.



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.

NCSP

NUCLEAR CRITICALITY SAFETY PROGRAM

NNSA

National Nuclear Security Administration

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

Thank you for your attention.

BACKUP: Other Past Benchmarks Used for ^{235}U Intermediate Evaluation

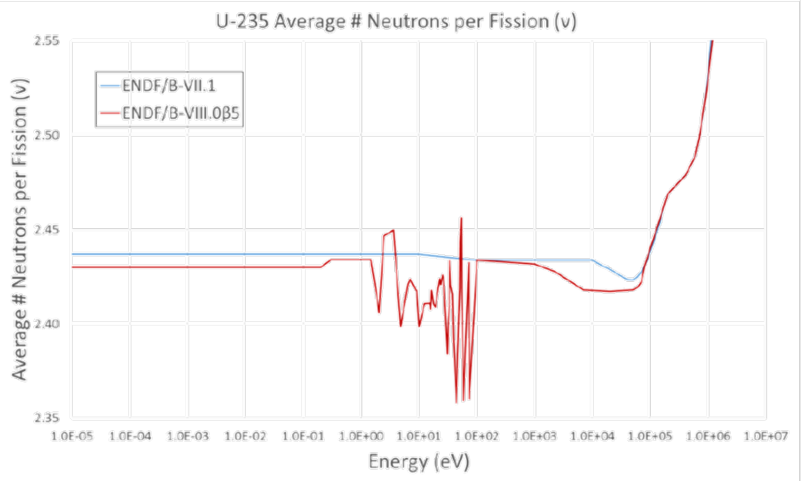
CSWEG KAPL Presentation (2017)
https://indico.bnl.gov/event/3580/contributions/10453/attachments/9386/11482/NNL_CSEWG_2017.pdf

HCI_003_04 Benchmark: Effect of ν

	E7.1	E7.1 + U-235 E8.0β5	Difference [%]
Capture ($\Sigma_\gamma\phi$)	2.094E-01	2.084E-01	-0.466
Leakage ($DB^2\phi$)	3.908E-01	3.889E-01	-0.470
Fission ($\Sigma_f\phi$)	3.998E-01	4.026E-01	+0.703
Nu (ν)	2.511	2.502	-0.351
Nu-Fission ($\nu\Sigma_f\phi$)	1.00383	1.00734	+0.349
k-eff (k)	1.00383	1.00734	+0.349

$$k = \frac{\nu\Sigma_f\phi}{\Sigma_\gamma\phi + \Sigma_f\phi + DB^2\phi} = \nu\Sigma_f\phi$$

Average neutrons per fission (nu) dropped from 2.511 to 2.502 between E7.1 and E8.0β5



- 409 pcm increase from:
  - Fe-56 ESAD/capture
  - U-235 capture/fission
  - U-235 ν

- HEU intermediate-spectrum models (HCI) are sensitive to changes in U-235 and O-16
  - nubar change has a 300-400 pcm affect

NAVAL NUCLEAR LABORATORY

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.