LA-UR-24-28948
Approved for public release; distribution is unlimited.

Title: Design and Development of IER:516 - Zirconium Test Assembly (ZTA) - Critical Experiments for Zr Nuclear Data Verification and Validation

Author(s): Siemers, Gregory Jay
Hutchinson, Jesson D.
Thompson, Nicholas William

Intended for: 2024 MCNP User Symposium, 2024-08-19/2024-08-22 (Los Alamos, New Mexico, United States)

Issued: 2024-09-17 (rev.1)

Design and Development of IER:516 – Zirconium Test Assembly (ZTA) – Critical Experiments for Zr Nuclear Data Verification and Validation

Gregory Siemers[1,2], Jesson Hutchinson[1], Nicholas Thompson[1]

[1]*Nuclear Engineering and Nonproliferation Division: Los Alamos National Laboratory – Los Alamos, NM, 87544*

[2]*Gaerttner LINAC Center: Rensselaer Polytechnic Institute – Troy, NY, 12180*

MCNP User Symposium - August 19-22, 2024
Los Alamos National Laboratory, Los Alamos, NM 87544

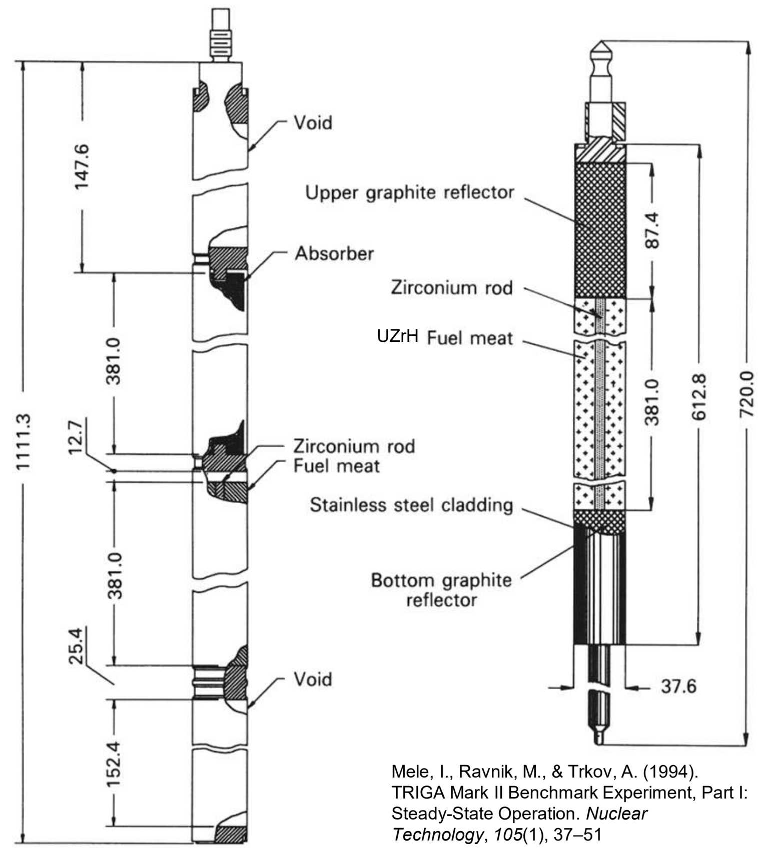
LA-UR-24-28948

Overview of IER:516 Zirconium Test Assembly (ZTA)

IER 516 is an experimental campaign funded by DOE-NCSP to produce and evaluate critical experiments for Zr metal and Zr Hydride nuclear data validation. **MCNP6 is being used as radiation transport code for design and development of configurations for the IER:516 experiments.**

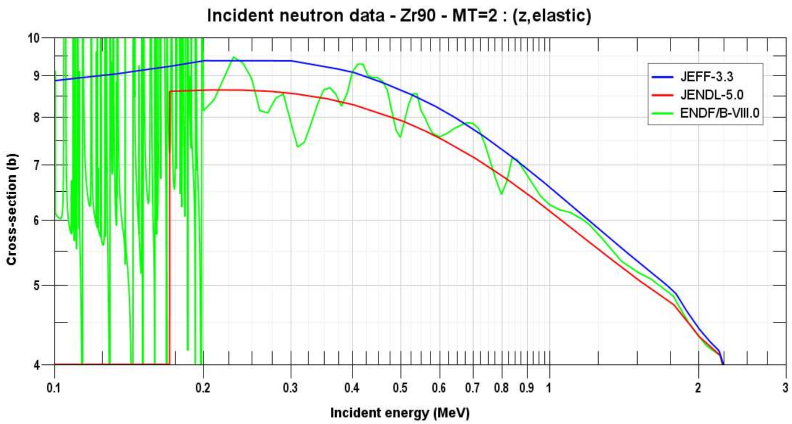
Motivation for Conducting Experiments:

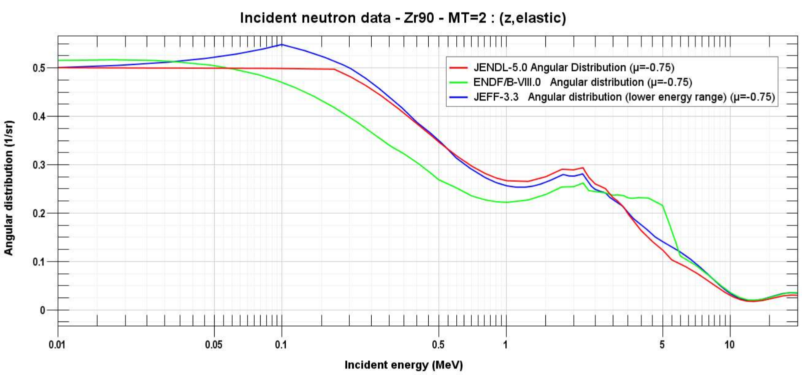
- Conflicts in evaluated and differential nuclear data
- Lacking isotopic differential nuclear data in regions of high importance to fission systems
  - Double differential elastic scattering below 1.5 MeV
- No experiments in ICSBEP optimized for Zr sensitivity

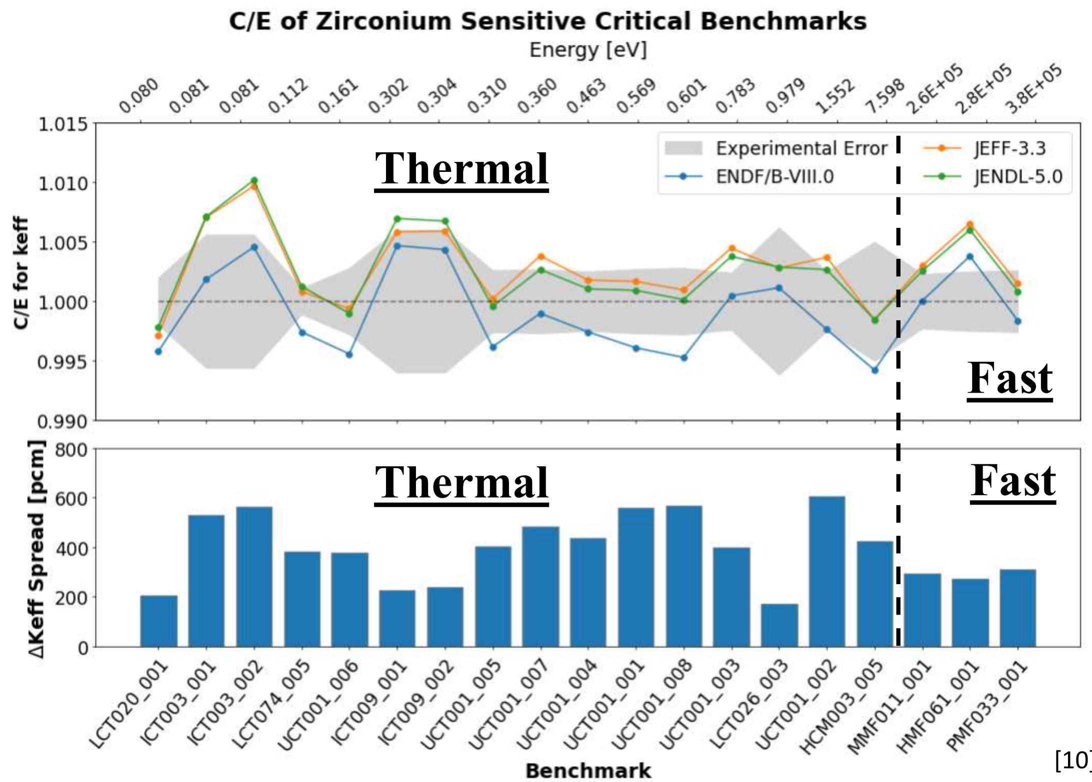


Mele, I., Ravnik, M., & Trkov, A. (1994). TRIGA Mark II Benchmark Experiment, Part I: Steady-State Operation. *Nuclear Technology*, *105*(1), 37–51

Conflicting Zirconium Nuclear Data



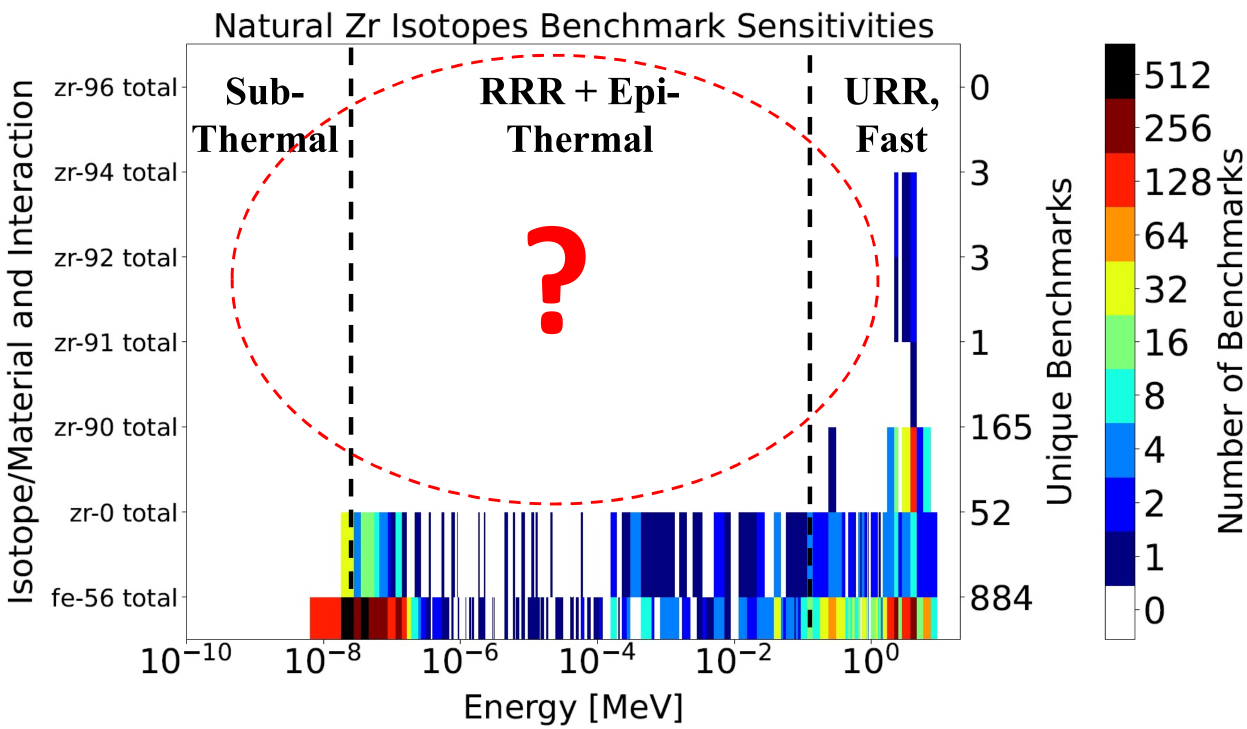




[10]

Lack of Zirconium Critical Benchmark Experiments

- High fidelity integral experiments are useful to validate performance of evaluated nuclear data
  - Most Zr sensitive benchmark experiments are large thermal systems with low, unintentional Zr sensitivity
  - Several do not meet modern ICSBEP evaluation standards



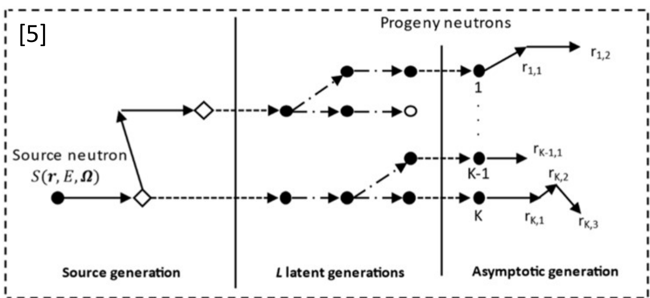
A score on this plot corresponds to a sensitivity coefficient greater than or equal to 1e-3 at a given energy [10]

Components of MCNP6 Used in Critical Experiment Design

MCNP-KCODE

- KCODE is a routine within MCNP6 which computes the time independent eigenvalue, or system K_{eff} of a multiplying nuclear system

[5]



KSEN

- Calculates sensitivity coefficients of a nuclear system to different nuclear data using the iterated fission probability methodology to compare adjoint-weighted flux tallies[6]

$$dk = -\frac{\langle \psi^{\dagger}, (d\Sigma_t - d\mathcal{S} - \lambda d\mathcal{F})\psi \rangle}{\langle \psi^{\dagger}, \lambda^2 \mathcal{F}\psi \rangle}, \qquad (1)$$

where

[6]

ψ = forward flux

$\psi^{\dagger}$ = forward flux adjoint

$\lambda = 1/k$

Σ_t = macroscopic total cross section

$\mathcal{S}$ = integral scattering operator

$\mathcal{F}$ = total integral fission operator

brackets = integration over all space, angle, and energy variables.

Flux Tallying

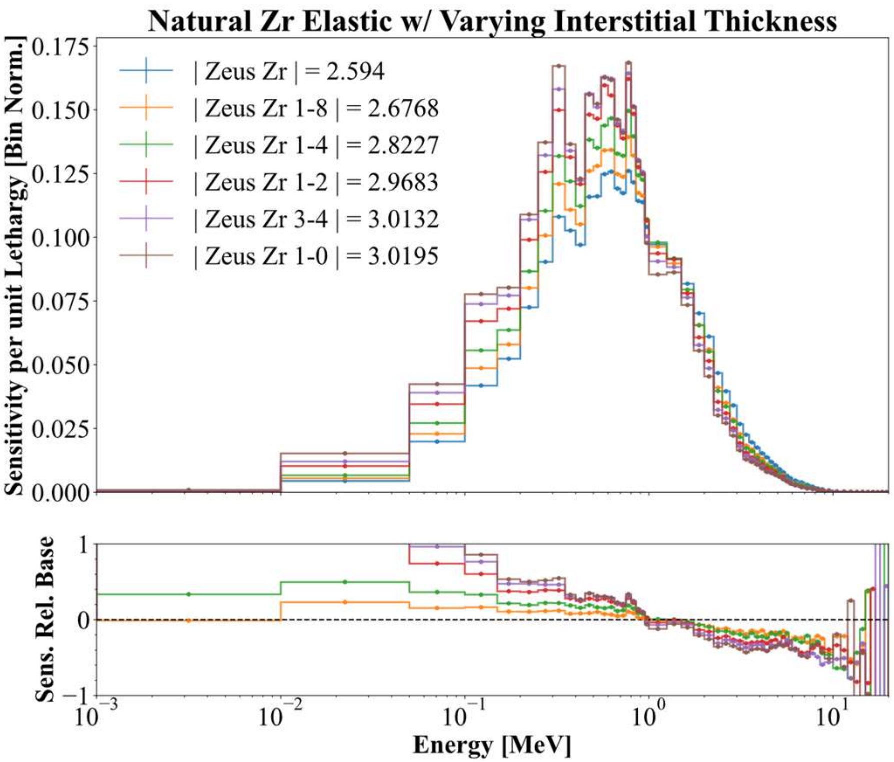
- Tallying the neutron flux averaged over cell(s) is very useful when designing criticality experiments
- Can obtain neutron spectrum throughout experimental assembly
- Can sample multigroup cross sections using tally modifier for calculations of ΔK_{eff}

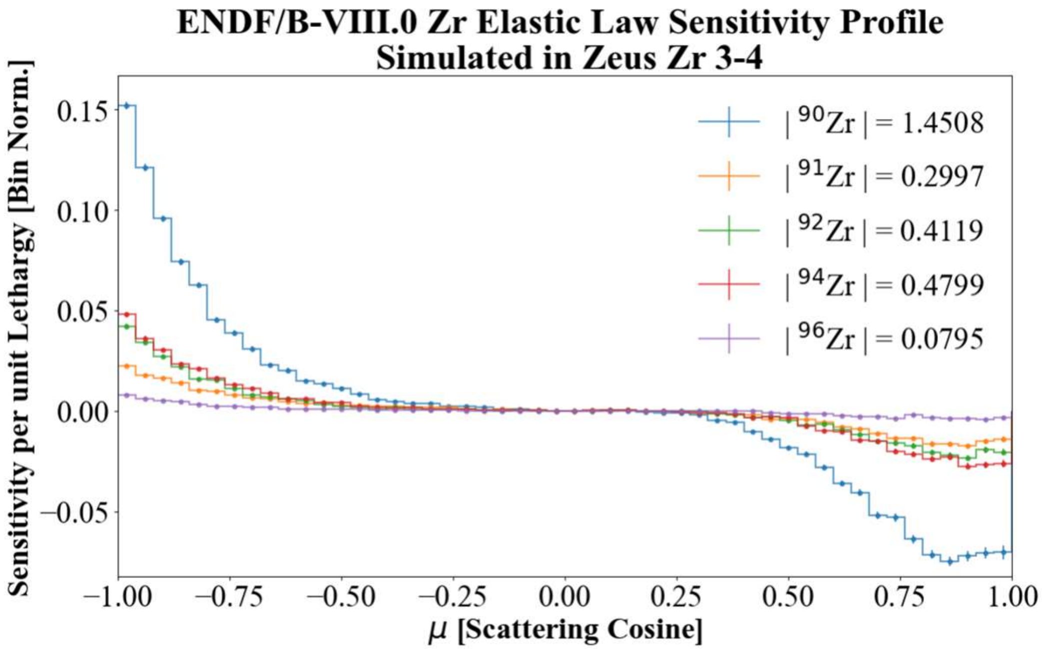
$$\mathrm{F4} = \frac{1}{V}\int_{E_i} \mathrm{d}E \int_{t_j} \mathrm{d}t \int \mathrm{d}V\, \phi(\mathbf{r}, E, t),$$

[7]

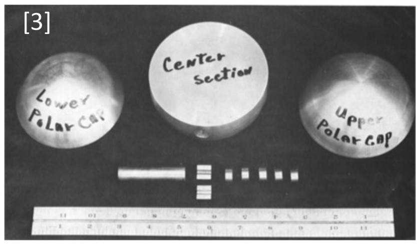
$$C\int \varphi(E) R_m(E) \mathrm{d}E,$$

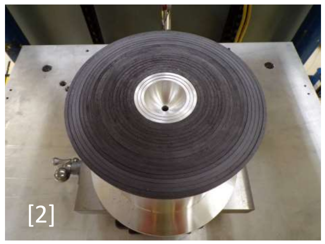
Examining Sensitivity Profiles of Potential Experiments

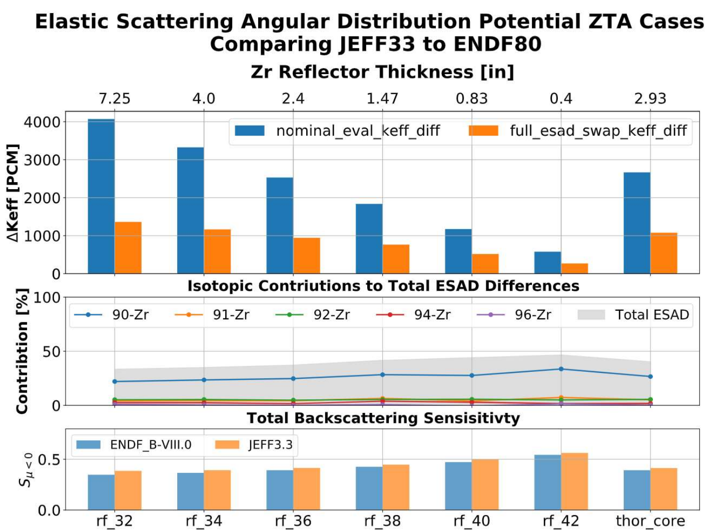


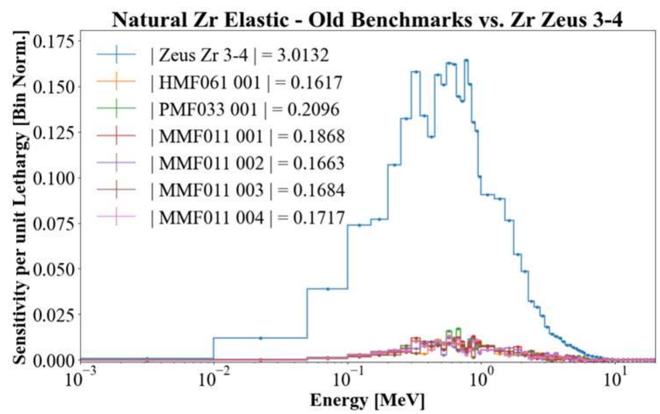


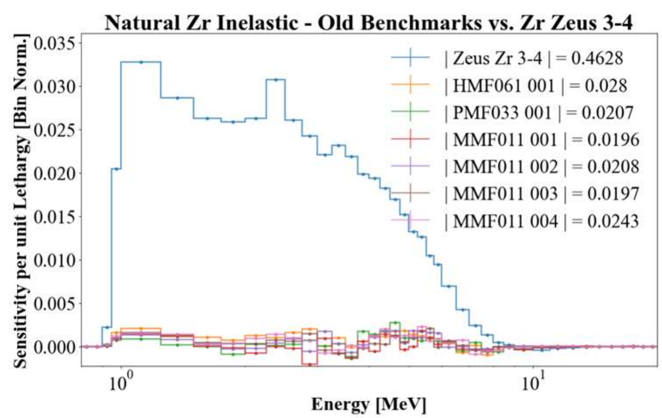
Development of Unmoderated Configurations





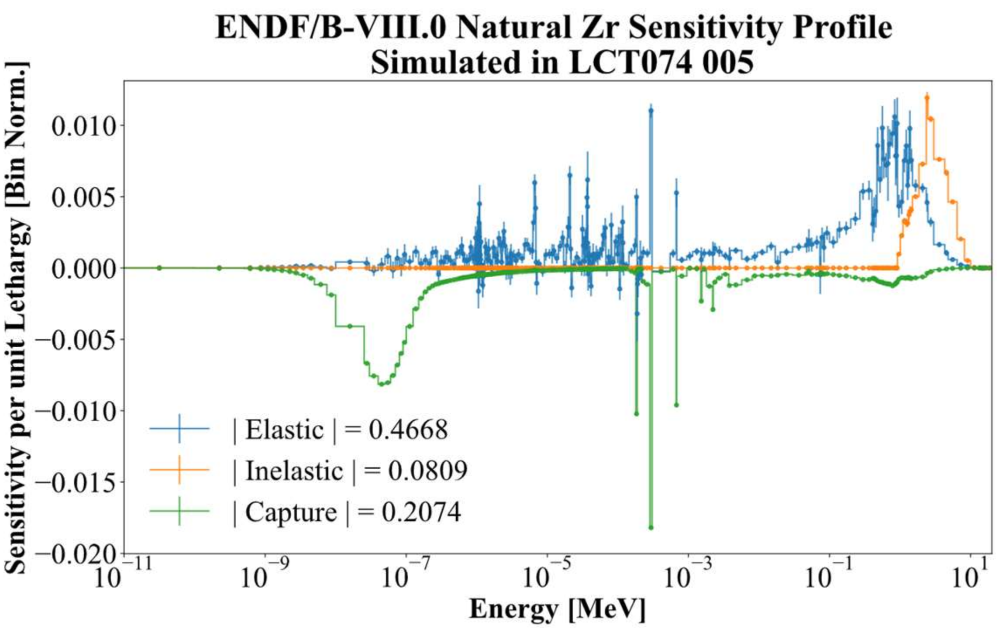


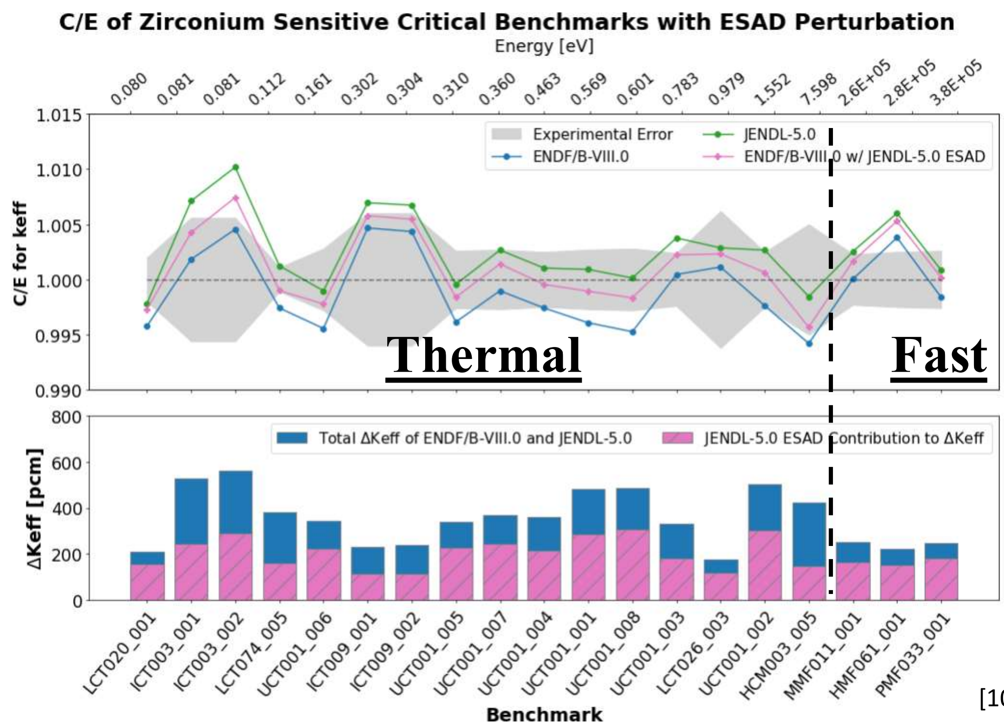




Why Emphasize Unmoderated Configurations?

But Zirconium is only used in thermal reactors…



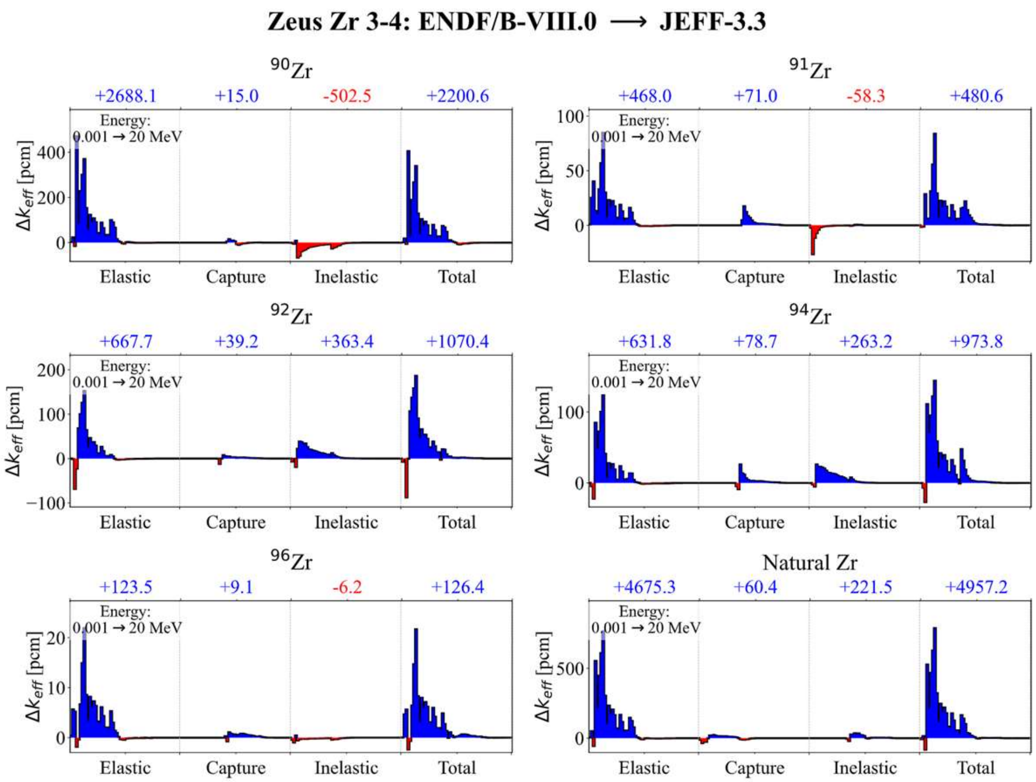


[10]

Using Sensitivity Profiles and Flux Tallying for More…

Relationship between sensitivity coefficients from MCNP KSEN and cross section differences from cell flux tallies (F4) can be used to propagate differences in cross sections between nuclear data evaluations to differences in the eigenvalues of simulated nuclear systems.

$$\Delta keff\left(\Sigma_i\,(E)\right) = \left[S_{keff}\left(\Sigma_i^{E8}(E)\right) * \left(\frac{\Sigma_i^{E8}(E) - \Sigma_i^{J33}(E))}{\Sigma_i^{E8}(E)}\right)\right] * keff(\Sigma_i^{E8}(E))$$



See more by Mike Rising and Jesson Hutchinson:

1. J. Hutchinson, et al. *EUCLID: A New Approach to Constrain Nuclear Data via Optimized Validation Experiments using Machine Learning,* EPJ Web of Conferences 284, 15006 (2023)
2. N. Thompson, et al. *The EUCLID Experiment and Nuclear Data Library Comparisons,* Conference: 12. International Conference on Nuclear Criticality Safety, Sendai (Japan), 1-6 Oct 2023
3. J. Hutchinson, et al. *EUCLID: Experiments Underpinned by Computational Learning for Improvements in Nuclear Data,* NCSP Annual Technical Program Review, Oak Ridge, TN 2022

Machine Learning to Narrow the Experiment Search Space

K - PSO

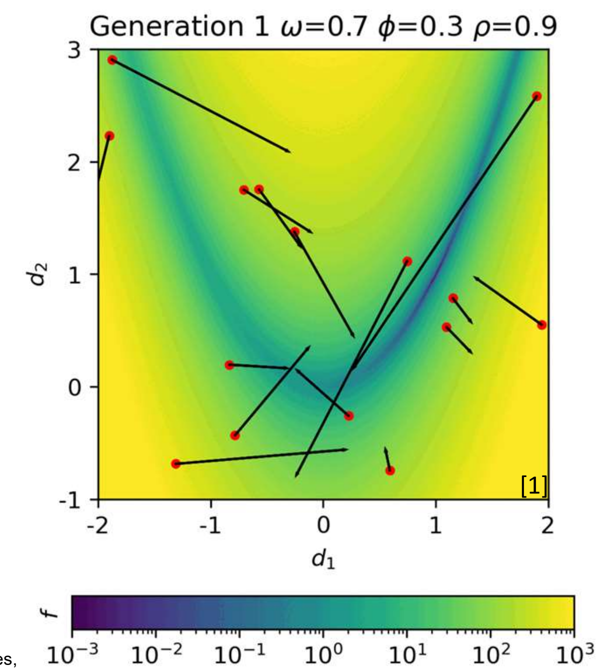
- Particle swarm optimization (PSO) algorithm coupled with MCNP6 through Python by C. Kostelac
- Used for CED-1 and CED-2 critical experiment designs (IER 517 and IER 551) – and now IER 516

$$\mathbf{v}_i^{k+1} = \omega \mathbf{v}_i^k + \phi r_1(\mathbf{p}_i^k - \mathbf{x}_i^k) + \rho r_2(\mathbf{g}^k - \mathbf{x}_i^k)$$ [8]

Previous velocity (inertia) — Particle best (cognitive) — Swarm best (social)

$$f(\mathbf{x}_i^k) = \begin{cases} |A| & 0.99 \le k_{eff} \le 1.01 \\ -|k_{eff} - 1| & otherwise \end{cases}$$ [8]

$$\frac{1}{S}\sum_{i=1}^{S} f(\mathbf{p}_i) > 0.95 f(\mathbf{g})$$ [8]



See more K-PSO materials:

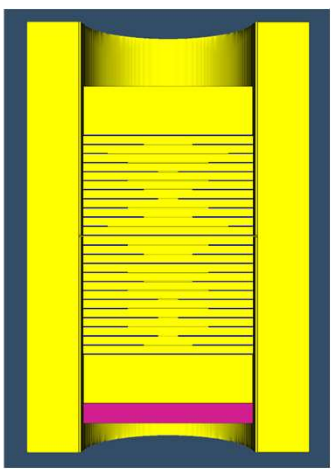
1. Kostelac, C: *Particle Swarm Optimization for Critical Experiment Design,* Master's Thesis Missouri University of Science and Technology ProQuest Dissertations & Theses, 2022
2. Kostelac, C. et al. *IER-517: Molybdenum Optimized Benchmark System Demonstrating Integral Correlations (MOBY DICK),* LA-UR-22-29826, 2022
3. Brain, P. et al. *IER-551: Experiment for Unresolved Resonance of Plutonium Actinides (EUROPA): CED-1 for True Intermediate Pu Benchmark,* LA-UR-23-24625, 2023

K-PSO for IER:516 Preliminary Design (CED-1)

Fast Cases

E_n > 500 keV

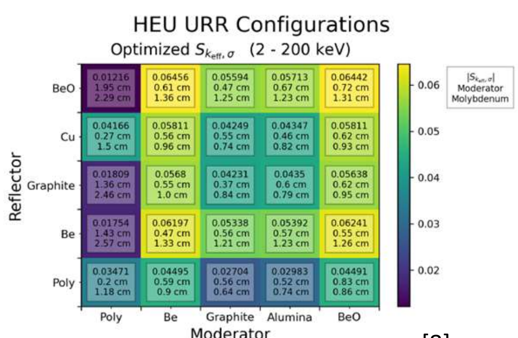
1. # unit cells
2. Zr interstitial thickness
3. Reflector thickness



Intermediate Cases

100 eV < E_n < 500 keV

1. Moderator material/thickness
2. Absorber material/thickness?
3. Exploit ^{91,96}Zr capture resonances and URR

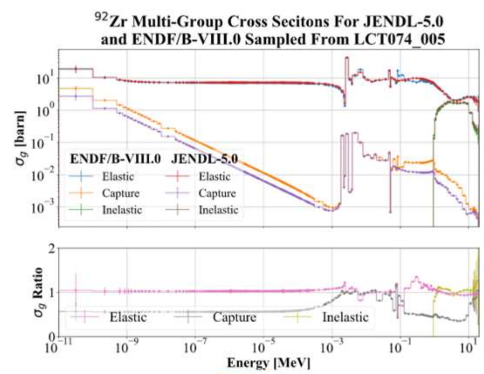


[8]

Epi/Sub/Thermal Cases

1e-5 eV < E_n < 100 eV

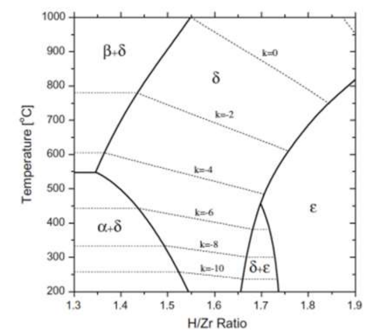
1. Exploit ^{91,92}Zr capture cross section differences between ENDF/B-VIII.0 and JENDL-5.0



Zirconium Hydride Cases

1e-5 eV < E_n < 100 eV

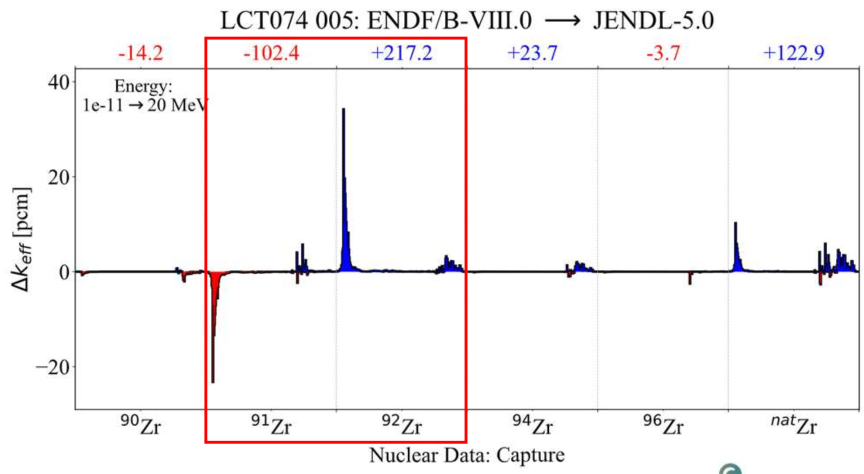
1. ZrH_x interstitial thickness
2. Zr metal interstitial thickness
3. Phase of ZrH_x moderator
4. Maximum possible Zr sensitivity



[9]

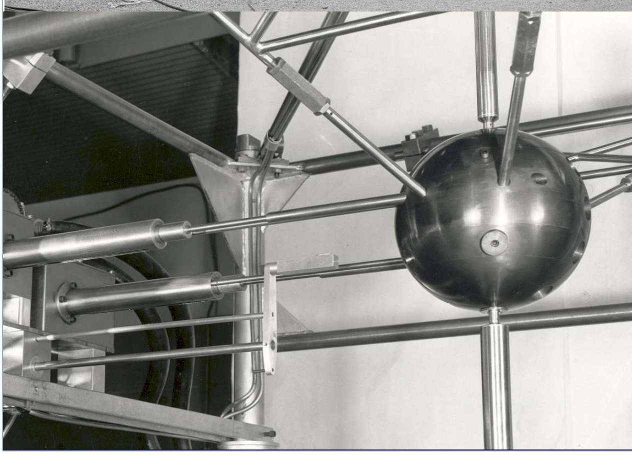
Implementation of New Features in K-PSO 2.0

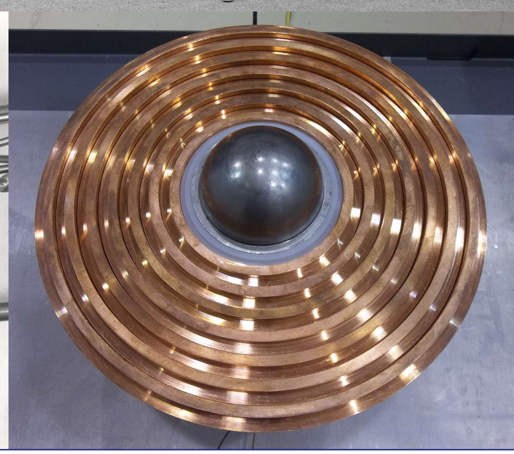
- Addition of maximization of a specific ΔK_{eff} value from previous methodology
  - Previously maximized/minimized only sensitivity, % fissions in energy region, or tally result
- Multi-node implementation on HPC systems
- Numerous quality of life and robustness updates
- This effort is still a work in progress



Final Remarks

- MCNP6 KCODE, KSEN, and tallying methods all integral to performing radiation transport simulations when designing and developing critical experiments
- Supplemental tools, such as the K-PSO program, have also been built to interface with MCNP6 to support the design of critical experiments
- Preliminary design (CED-1) of critical experiments for IER-516: Zirconium Test Assembly is underway using MCNP6
  - New configurations yield over an order of magnitude increase in sensitivity to Zr
  - Enormous differences in eigenvalue calculation between evaluated nuclear data libraries observed





Los Alamos
NATIONAL LABORATORY

Questions?

Rensselaer

linac The Gaerttner LINAC Center

NCSP NUCLEAR CRITICALITY SAFETY PROGRAM

NCERC

NNSA National Nuclear Security Administration

Acknowledgement

This work is sponsored by the Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the U.S. Department of Energy.

Additional References

1. Kostelac, C. *IER:517 MOBY DICK CED-1 Overview,* Nuclear Criticality Safety Program Annual Technical Program Review, 2023
2. Ogren, K. *IER 488: MUSIC: Reactivity Estimates using Pulsed Neutron Source Methods,* Nuclear Criticality Safety Program Annual Technical Program Review, 2023
3. Hansen, G. and Paxton, H. *Thor, A Thorium-Reflected Plutonium-Metal Critical Assembly,* Nucl. Sci. Eng. **71**, 287-293 (1979)
4. Goetta, J. *LANL FY22 NCSP Highlights,* Nuclear Criticality Safety Program Annual Technical Program Review, 2023
5. Tuya, D. and Nagaya, Y. *Estimation of Continuous Distribution of Iterated Fission Probability Using an Artificial Neural Network with Monte Carlo-Based Training Data,* J. Nucl. Eng. (2023), 4 (4), 691-710
6. Kiedrowski, B. and Brown, F. *Adjoint-Based k-Eigenvalue Sensitivity Coefficients to Nuclear Data Using Continuous-Energy Monte Carlo,* Nucl. Sci. Eng., 173:3, 227-224 (2017)
7. Rising, M. et al. *MCNP Code Version 6.3 Theory & User Manual,* LA-UR-22-30006, Rev. 1 (2022)
8. Kostelac, C: *Particle Swarm Optimization for Critical Experiment Design,* Master's Thesis Missouri University of Science and Technology ProQuest Dissertations & Theses, 2022
9. Hu, X. et al. *Technology Enabling Zero-EPZ Micro Modular Reactors - Milestone M2.2.2 - Fabrication of Zirconium Hydride with Controlled Hydrogen Loading*, ORNL/SPR-2020/1672, https://info.ornl.gov/sites/publications/Files/Pub146553.pdf (2020)
10. Siemers, G. *New Zirconium Evaluations for ENDF/B-IX,* Mini-CSEWG Annual Meeting, Los Alamos, NM, August 2024