TOWARDS TSL UNCERTAINTY

The TARA project

AMWG meeting 2026

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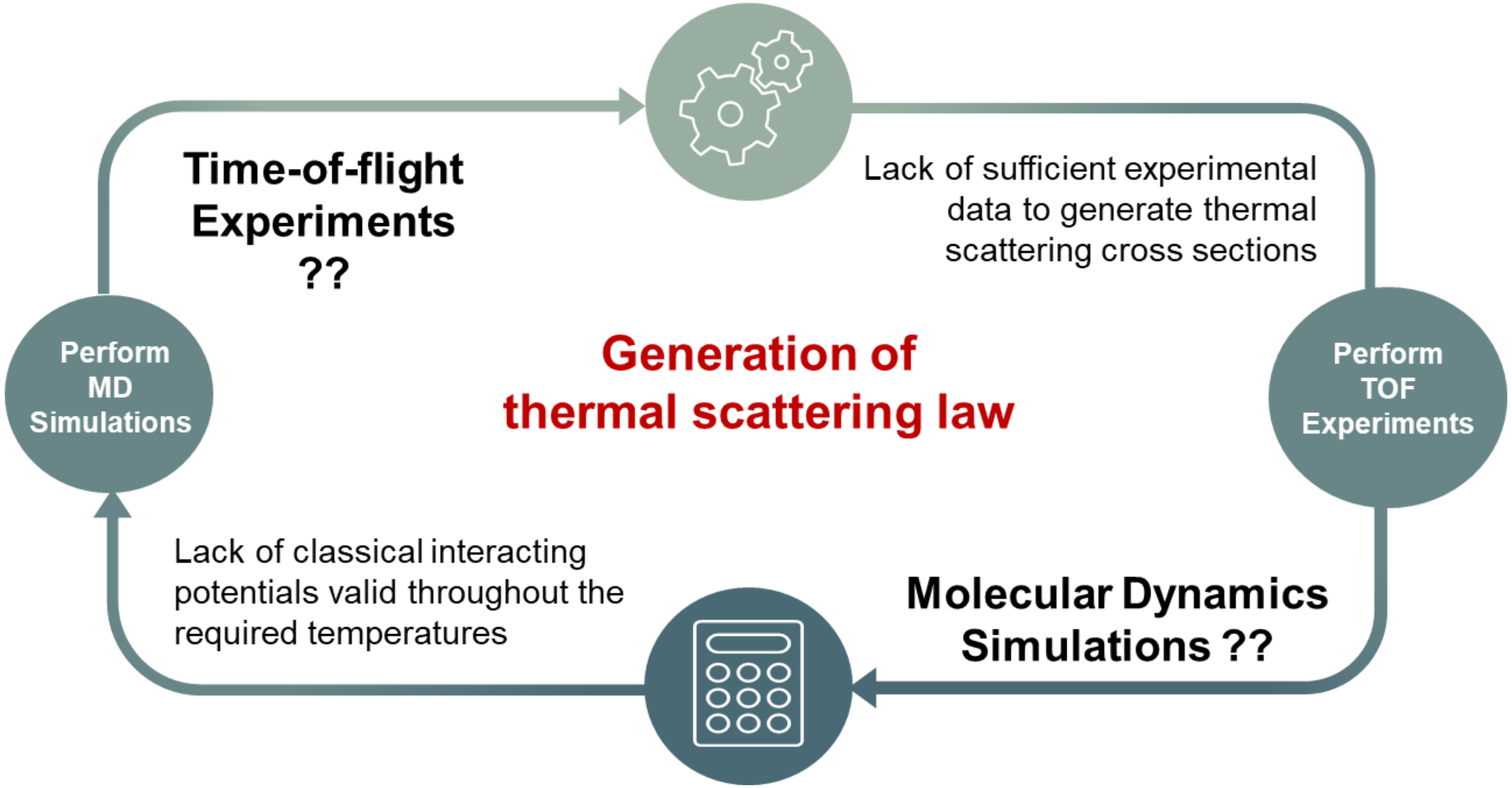
PSN-RES/SNC/LN

WHAT DO WE HAVE TODAY ?

Neutron thermalization in nuclear systems depends critically on accurate thermal scattering cross sections, which are governed by the **Thermal Scattering Law (TSL).**



Existing No. Of TSLs in ..

JEFF-4.0	ENDF/B-VIII.1
TSL: ~ **80**	TSL: ~ **110**

- No available covariance matrix or uncertainty information on TSLs in any nuclear data library !
- Generating TSL covariances are complex and more work is needed !
- Uncertainty in TSLs impacts reactor simulations, benchmarks, safety margins !

WHAT DO WE HAVE TODAY ?

Academic contributions (PhDs) in recent years ..

Thesis	Author	Status / Year
Analytical Developments of Thermal Scattering Models: Doppler Broadening with CLM and Up-scattering in the Resonance Range	Aitor Bengoechea Fernández (CEA, France)	**Defended October 2025**
Nuclear Data Uncertainties Processing and Propagation	Pierre Solé (ASNR, France)	**Defended November 2025**
Measurement of the Double Differential Neutron Cross Section of UO_2 and Determination of the Thermal Scattering Law as a Function of Temperature	Shuqi Xu (CEA, France)	2021
Thermal Scattering Law Uncertainties and Propagation into Small Thermal Fission Reactors	Lance Maul (UNSW, Australia)	2018
Amélioration des données neutroniques de diffusion thermique et épithermique pour l’interprétation des mesures integrals	Juan Pablo Scotta (CEA, France)	2018
From Experiments to DFT Simulations: Comprehensive Overview of Thermal Scattering for Neutron Moderator Materials	Kemal Ramić (RPI, US)	2018
Theoretical and Experimental Approach Towards Generation of Thermal Scattering Law for Light Water	Vaibhav Jaiswal (IRSN, France)	2018
Thermal Neutron Scattering Evaluation Framework	Chris W. Chapman (ORNL, US)	2017

ONGOING WORK AT ASNR | EXAMPLE: TSL FOR WATER

NUCLEAR SCIENCE AND ENGINEERING

DOI: https://doi.org/10.1080/00295639.2025.2530301

Check for updates

An Optimization Approach to Improve Thermal Scattering Law Using Experimental Total Cross-Section Data

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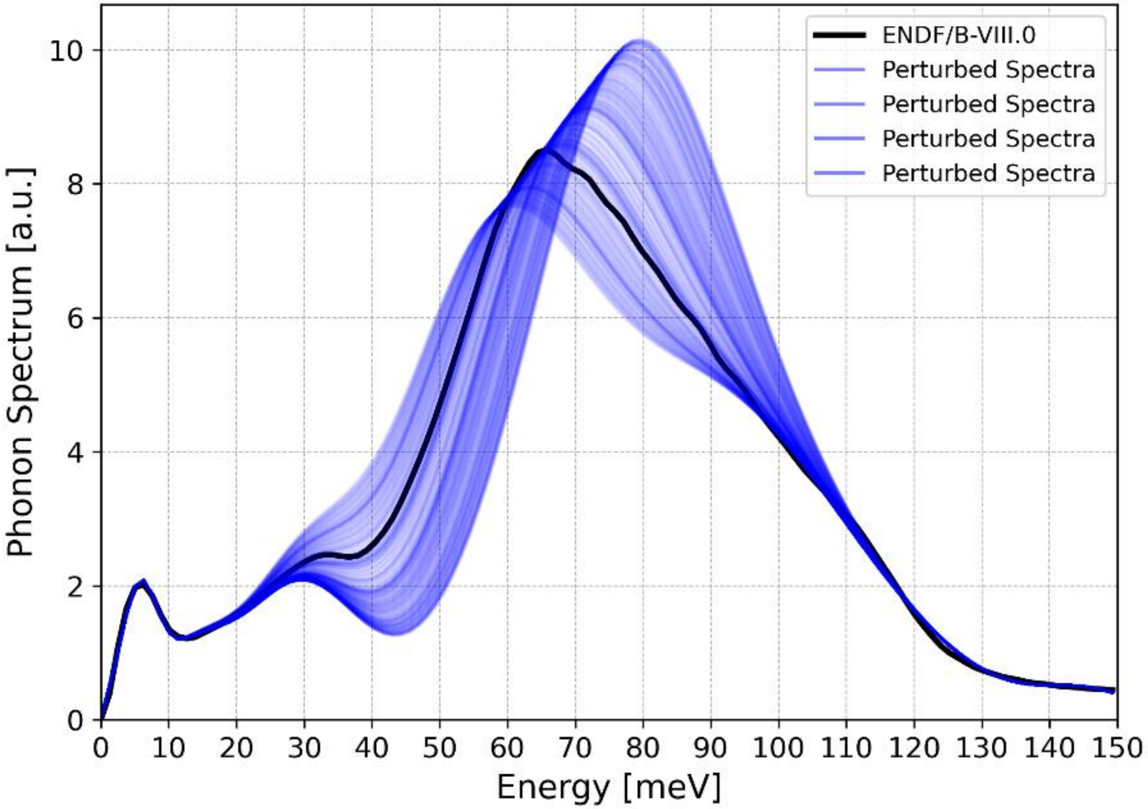
Received August 16, 2024
Accepted for Publication July 1, 2025

Abstract — *This paper presents a systematic optimization approach to improve the thermal scattering law (TSL) for light water by integrating experimental total cross-section data from the EXFOR database. The methodology is based on a chi-square minimization technique that adjusts the underlying phonon spectrum and discrete oscillator parameters in the LEAPR framework of the NJOY code. A detailed analysis of various perturbed phonon spectra was conducted, leading to the identification of optimized parameters that minimize discrepancies between the calculated and experimental cross section over the energy range of 0.1 to 500 meV.*

The optimized TSL evaluation demonstrated improved agreement with experimental data, reducing the mean absolute deviation from approximately 2.99% to 2.77%. Additionally, a preliminary correlation matrix is introduced to assess the interdependencies between different energy bins, offering insights into uncertainty quantification. Furthermore, validation of the optimized TSL against selected International Criticality Safety Benchmark Evaluation Project benchmarks confirms its enhanced predictive capability for reactor physics and criticality safety applications.

The framework developed in this study provides a robust methodology for refining TSL evaluations for light water through a computationally efficient workflow leveraging parallelized GAIA processing and lays the groundwork for extending these optimization strategies to other moderator materials.



ONGOING WORK AT ASNR

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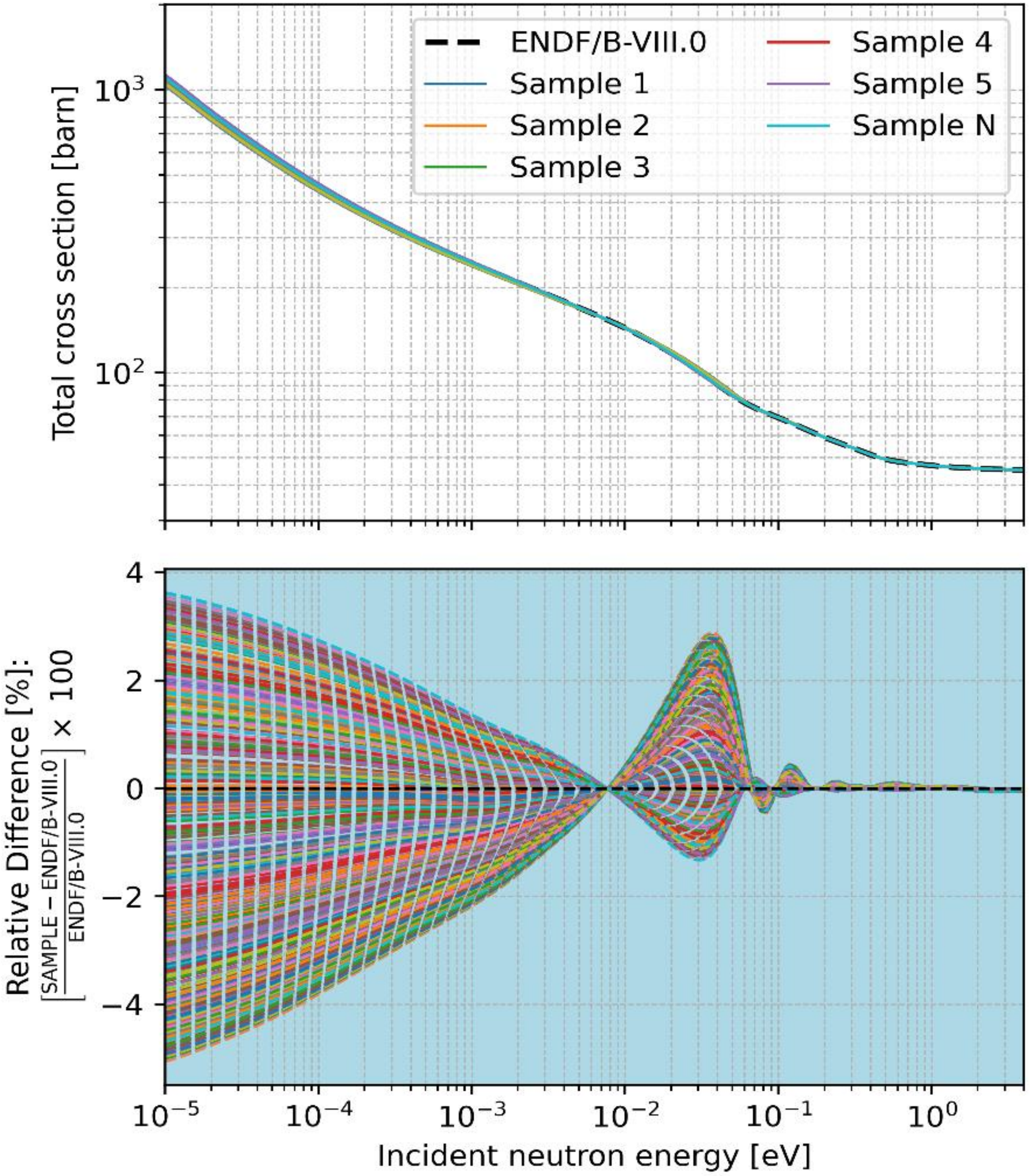
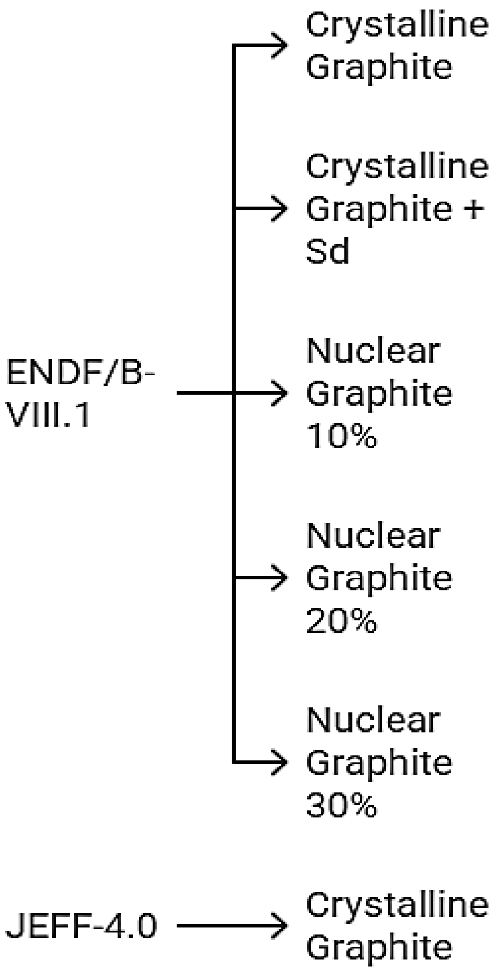


ONGOING WORK AT ASNR | EXAMPLE: TSL FOR GRAPHITE

Graphite TSL evaluations currently included in standard nuclear data library:



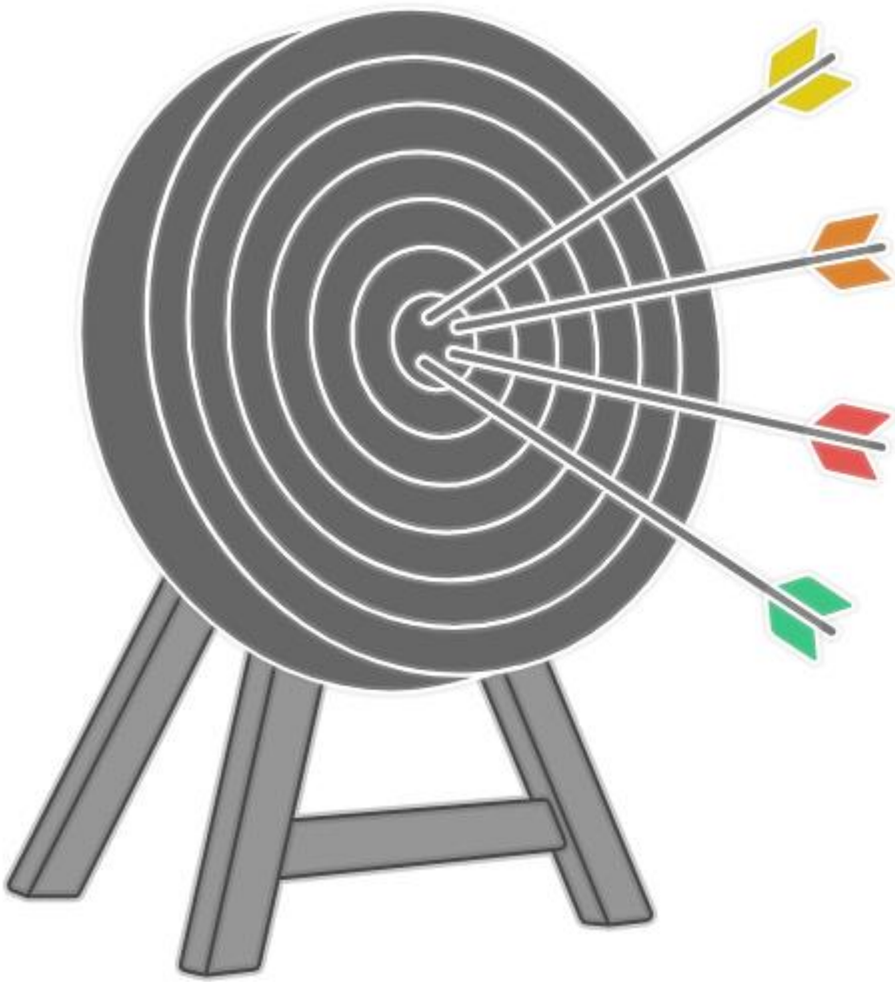
Property	ENDF/B-VIII.1	JEFF-4.0
Crystalline Graphite	Yes	Yes
Nuclear Graphite	Yes	No
Porosity	0%, 10%, 20%, 30%	Not specified

Some questions :

- Which TSL (among all available : for Graphite) to use?
- Benchmarks sensitive to TSL for Graphite?
- Will we have benchmarks dependent TSL?
- **Bigger question: What is the uncertainty on these TSL?**
- **Several competing TSL recommendation for Graphite in the literature.**

COMPETING TSL RECOMMENDATIONS: GRAPHITE

Recommendation [1]:



Recommended TSL

Crystalline Graphite (+Sd correction) (Sd-graphite)

Justification

The Phonon spectrum of different graphite shows excellent agreement with crystalline graphite, regardless of porosity.

Modeling Principle

Porosity is fundamentally a macroscopic effect (changing density) and should have no impact on the neutronics (K_{eff}).

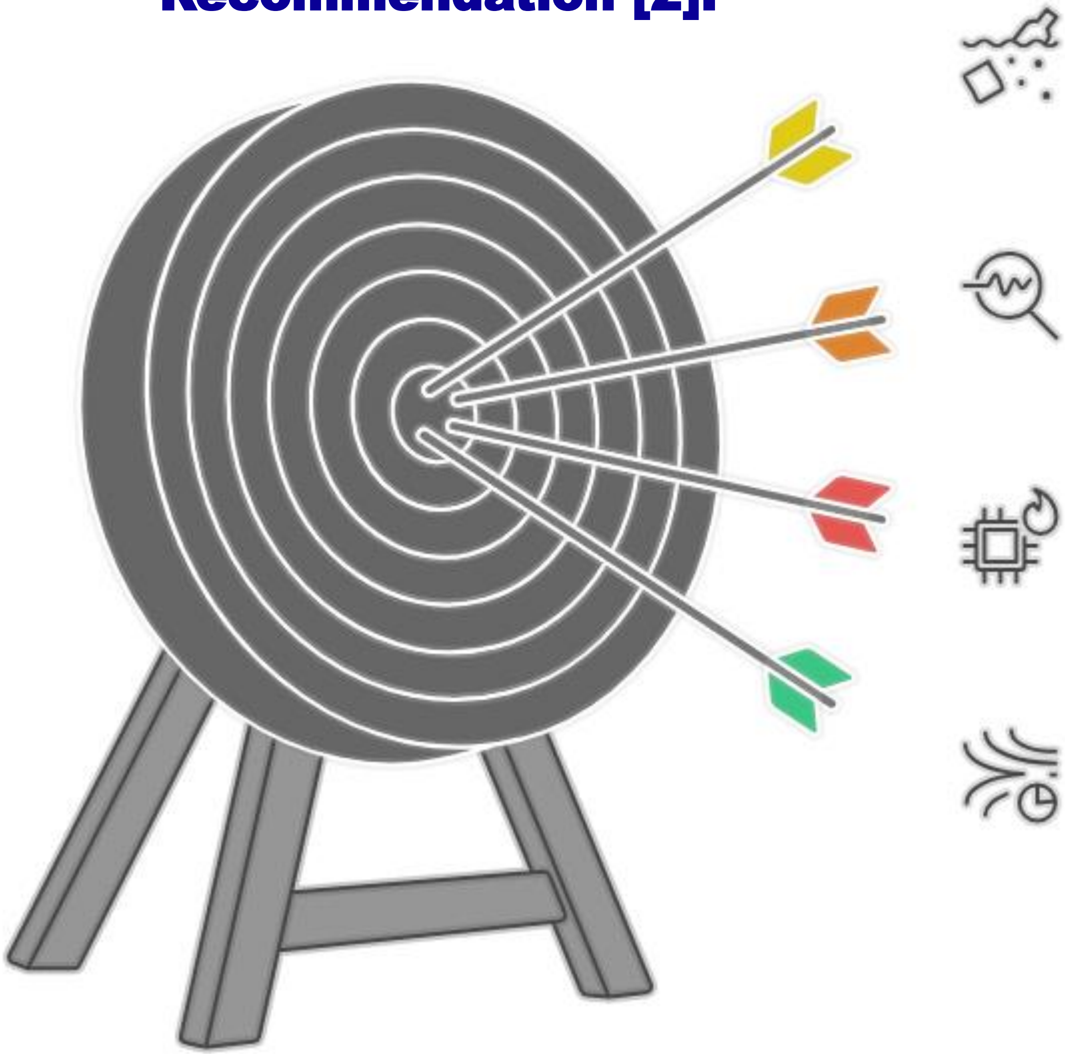
Critique of Porous TSLs

Porous TSLs increase the K_{eff} due to altered, unphysical inelastic scattering introduced by random atom removal.

[1] Iyad Al-Qasir, Graphite Thermal Neutron Scattering: Advancing from Basic Principles to Criticality Insights, NCSP TPR meeting, 2024.

COMPETING TSL RECOMMENDATIONS: GRAPHITE

Recommendation [2]:



Recommended TSLs

Porous Nuclear Graphite TSLs (e.g., 20% or 30% porosity)

Justification

Porous TSLs significantly improve agreement in key integral benchmarks

Validation

- The 30% Porous TSL evaluation improves validation with ORELA benchmark
- The 20% Porous TSL improves the PROTEUS benchmark

Modeling Principle

The neutron "samples everything in the bulk". Porous TSL model attempts to represent the homogenized bulk

[2] Ayman Hawari, Thermal Scattering Law Research and Development at NC State University, NCSP TPR meeting, 2024.

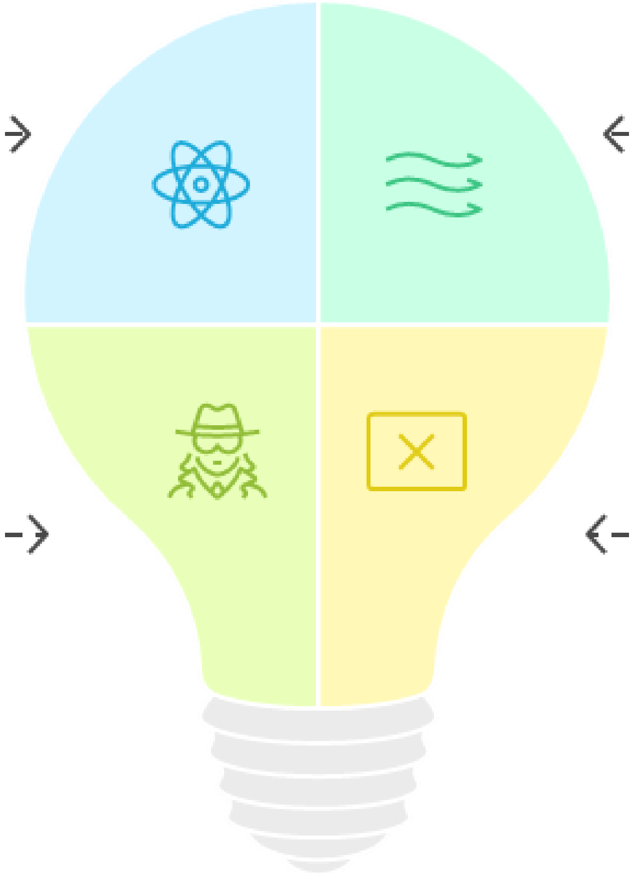
ONGOING WORK AT ASNR : THE TARA PROJECT

The TARA project helps answer these questions on quantifying the uncertainties in TSLs

TARA:
Thermal scattering law
uncertainty **A**nalysis using
RAndom files

PostDoc Recruited:
Aitor FERNANDEZ
BENGOECHEA

Started in November 2025 at
ASNR



EU project:
APRENDE
Task 4.2
Thermal neutron
scattering

Participation:
Gilles NOGUERE (CEA)
Jose Ignacio MÁRQUEZ DAMIÁN (ESS)
Mathieu HURSIN (EPFL)
Participants welcome to join !

TARA

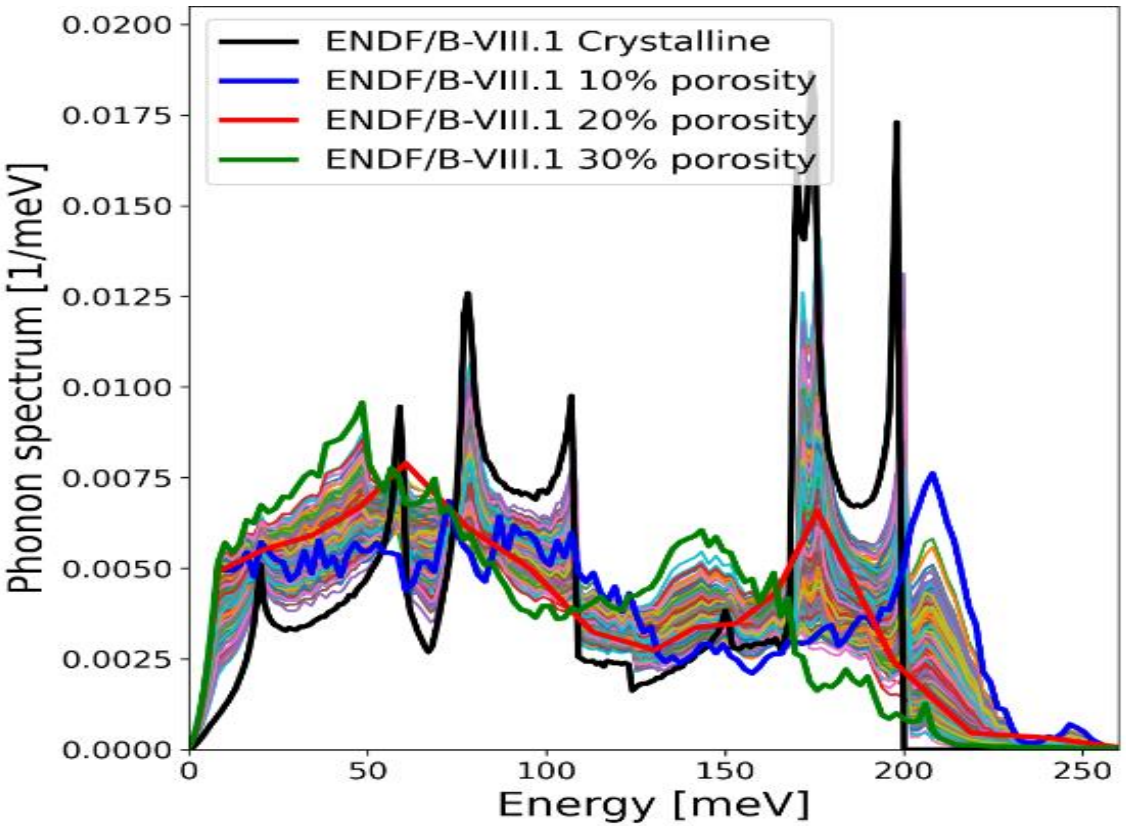
- This task will provide a ready-to-use tool for generating random TSL files for moderator materials.
- The main objective of TARA is to propose a methodology for quantifying TSL uncertainties.
- ASNR will be involved in the development, testing, and validation of this tool, in collaboration with CEA and ESS.
- The generated TSL samples should be realistic, as the sampling in TARA is constrained by available experimental and simulation data to ensure consistency with observable measurements (phonon spectrum, specific heat capacity, diffusion coefficients, etc).
- TARA helps in understanding how parameter uncertainties propagate through the cross sections, guiding subsequent optimization strategies.
- At the user level, TARA answers the question: *What is the impact on K_{eff} when using a particular TSL for criticality safety and reactor benchmarks?*

TARA: GRAPHITE TSL

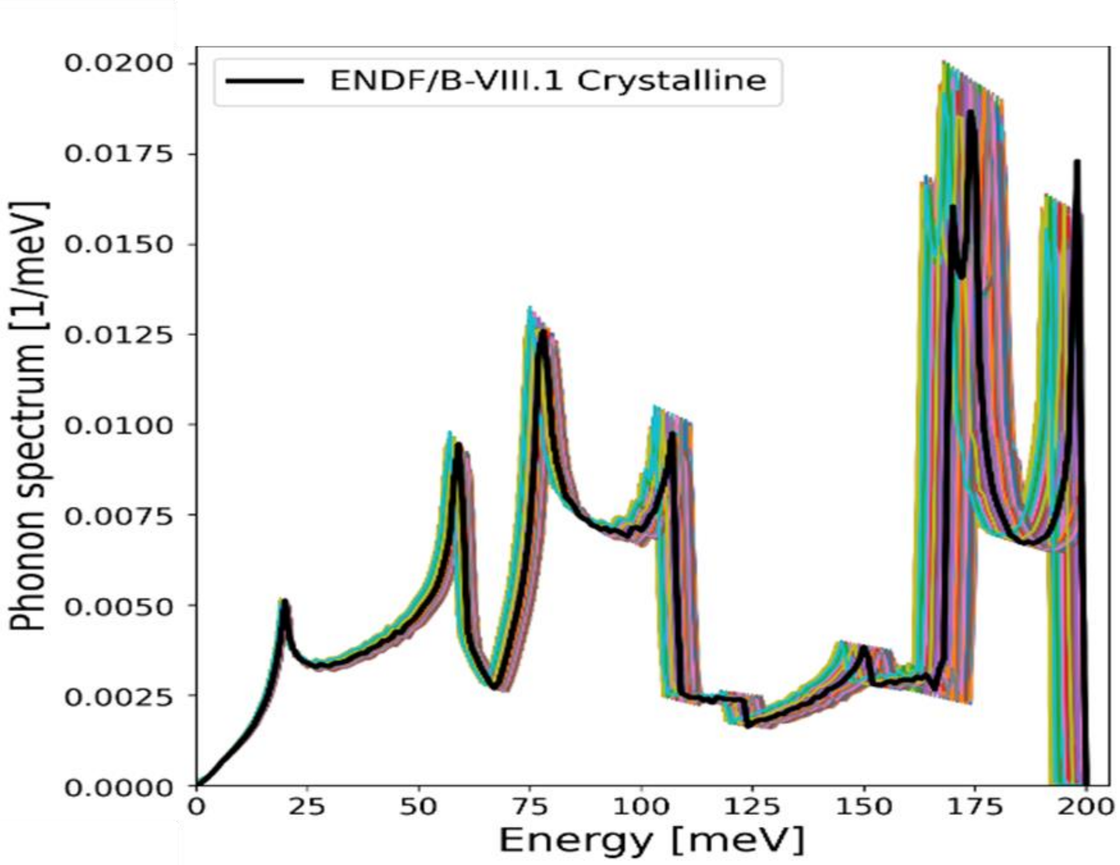
```
ARGS=(
    # --- Positional Input ---
    "tsl-crystalline-graphite.leapr"      # The main template LEAPR file

    # --- General Options ---
    "--mode" "gen"                        # Activate generative mode
    "--output_dir" "samples"              # Directory where results are saved
    "--n_samples" "500"                   # Total number of samples to generate

    # --- Reference Data ---
    # List all reference files used to learn the variance/shapes
    "--reference_files"
    "tsl-reactor-graphite-10P.leapr"      # Ref 1: 10% Porosity
    "tsl-reactor-graphite-30P.leapr"      # Ref 2: 30% Porosity

    # --- Strategy Configuration ---
    "--strategy" "cv"                     # CV: Convex Combination method
    "--sampler" "global"                  # Global: Use all loaded data
)
```

- A command-line tool.
- Example: Use Crystalline graphite (ENDF/B_VIII.0) at 293.6 K as reference TSL.
- Two reference uncertainty data (let’s assume it to be an independent experimental/simulation data) that guides the uncertainty on the graphite TSL.
- Here 10% and 20% data is taken as uncertainty guide data.
- Generate **500 random TSL evaluations.**

TARA: GRAPHITE TSL | SAMPLING STRATEGY



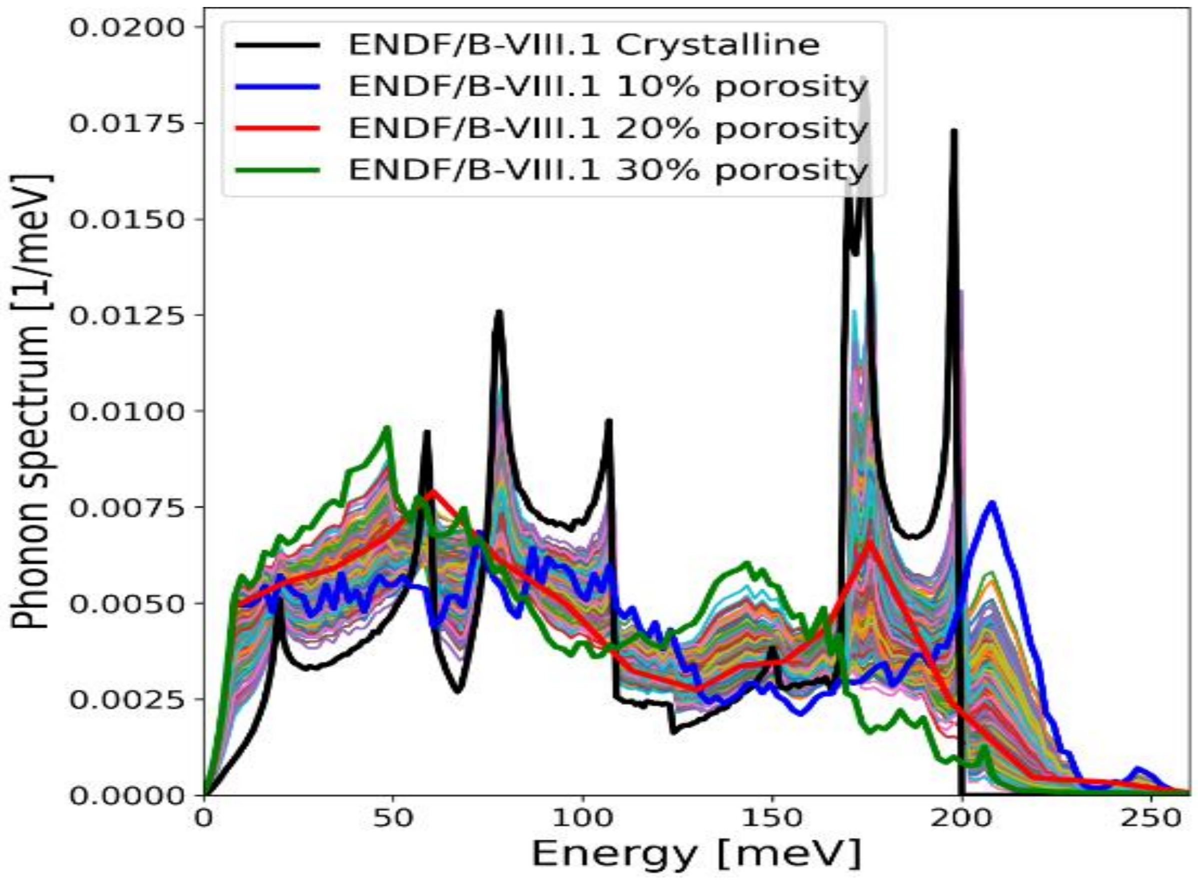
Strategy 1: **Blind sampling using various Graphite TSLs available in ENDF/B-VIII.1 (Crystalline, 10% porosity, 20% porosity, etc..)**

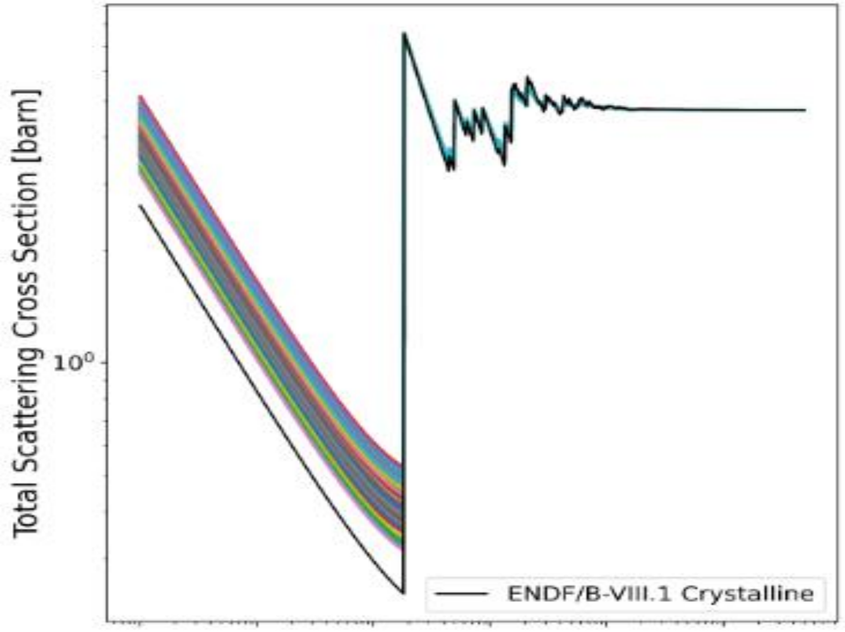


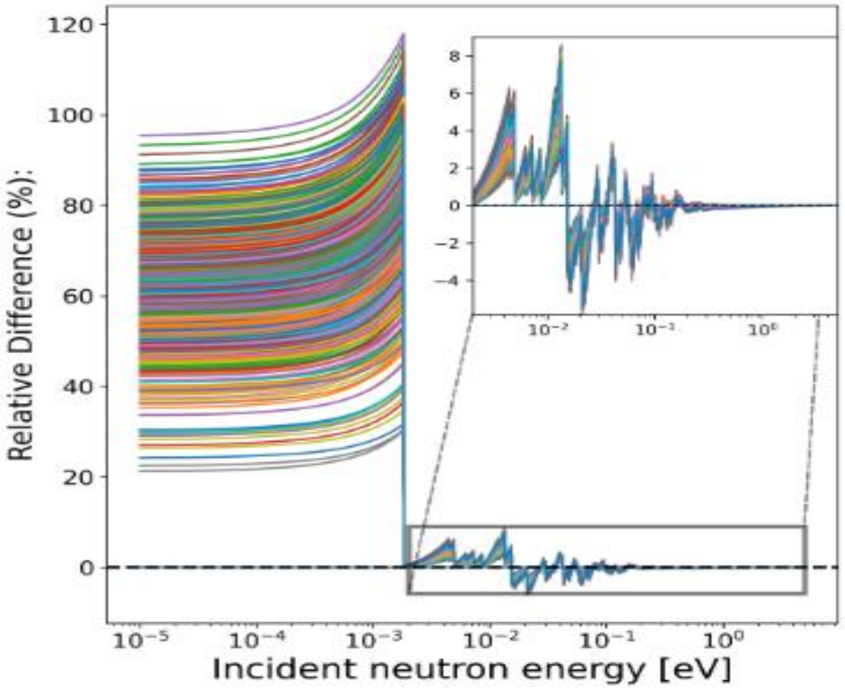
Strategy 2: **Restricted sampling using the Crystalline graphite TSL available in ENDF/B-VIII.1 (peak position perturbation)**

TARA: GRAPHITE TSL | SAMPLING 1

Blind sampling using various Graphite TSLs available in ENDF/B-VIII.1 (Crystalline, 10% porosity, 20% porosity, etc..)

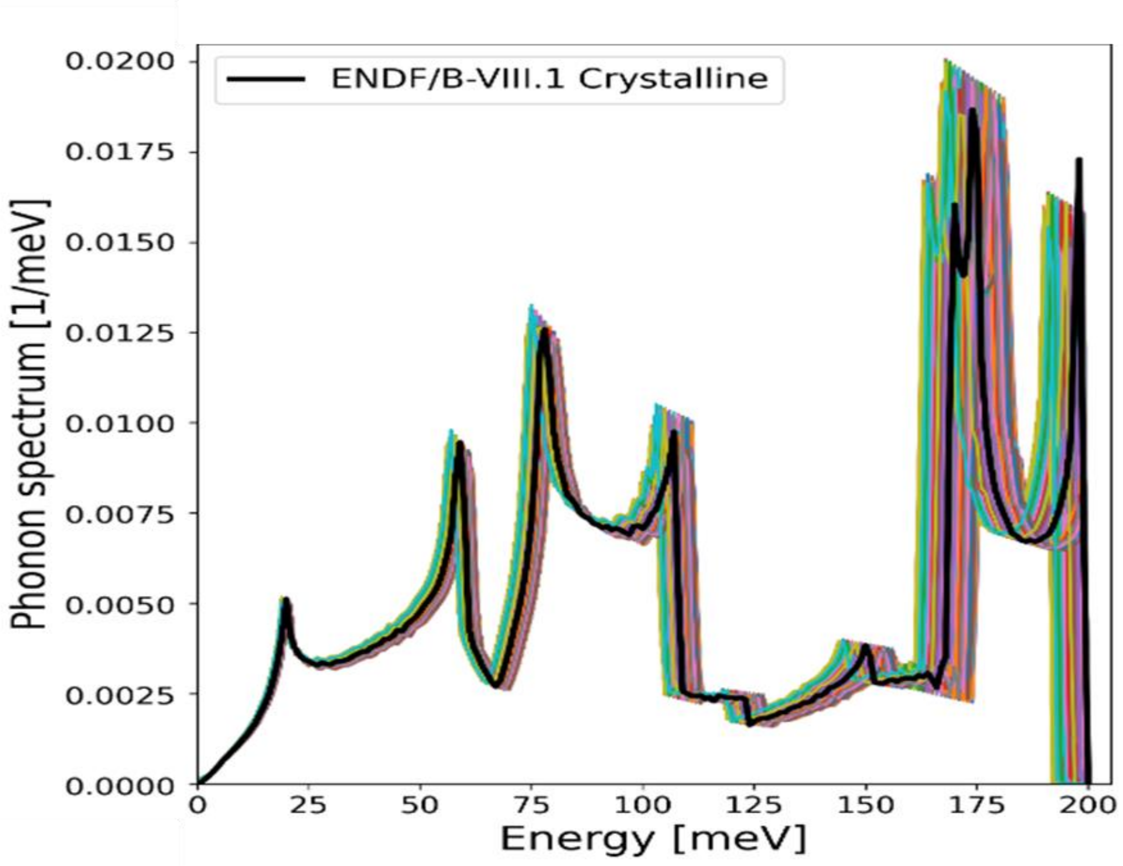


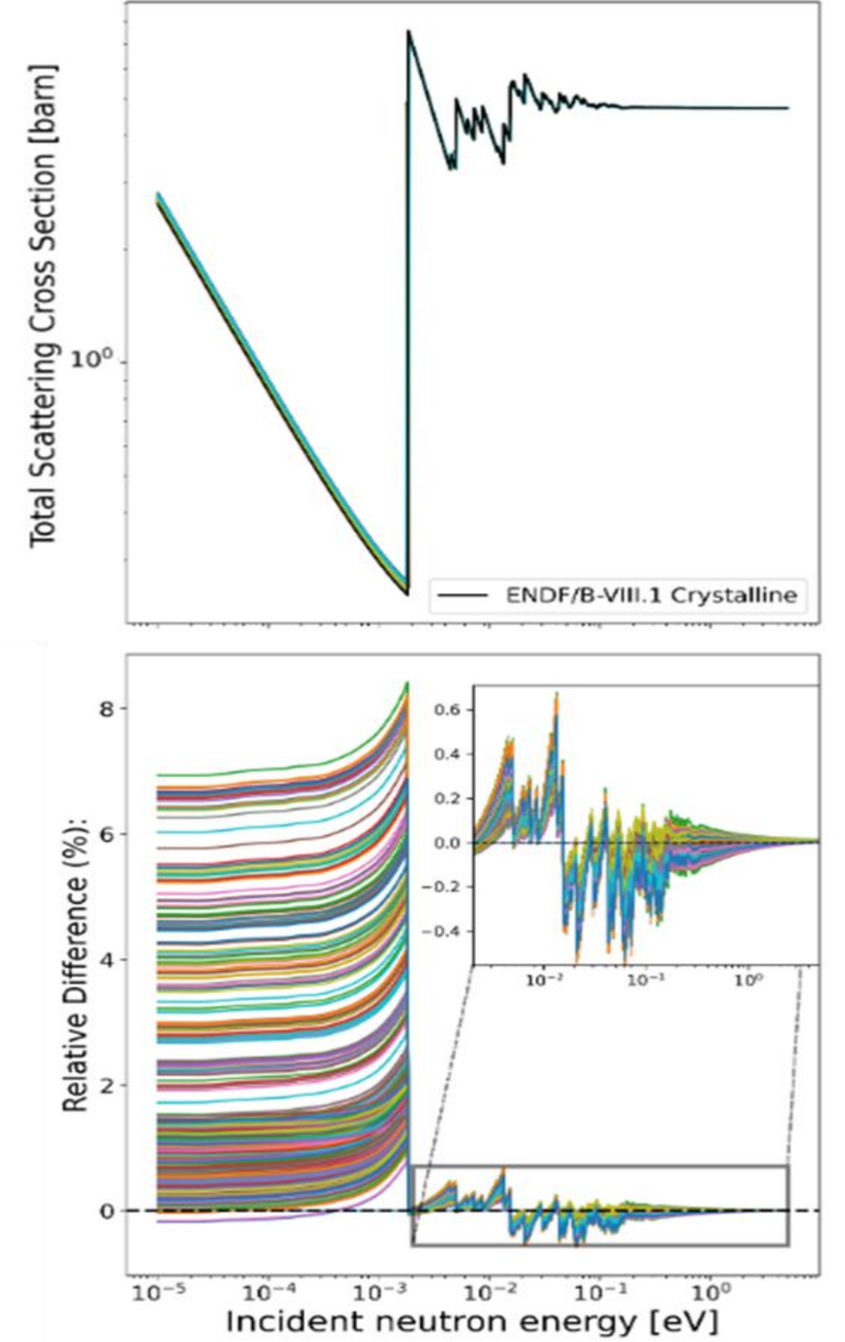




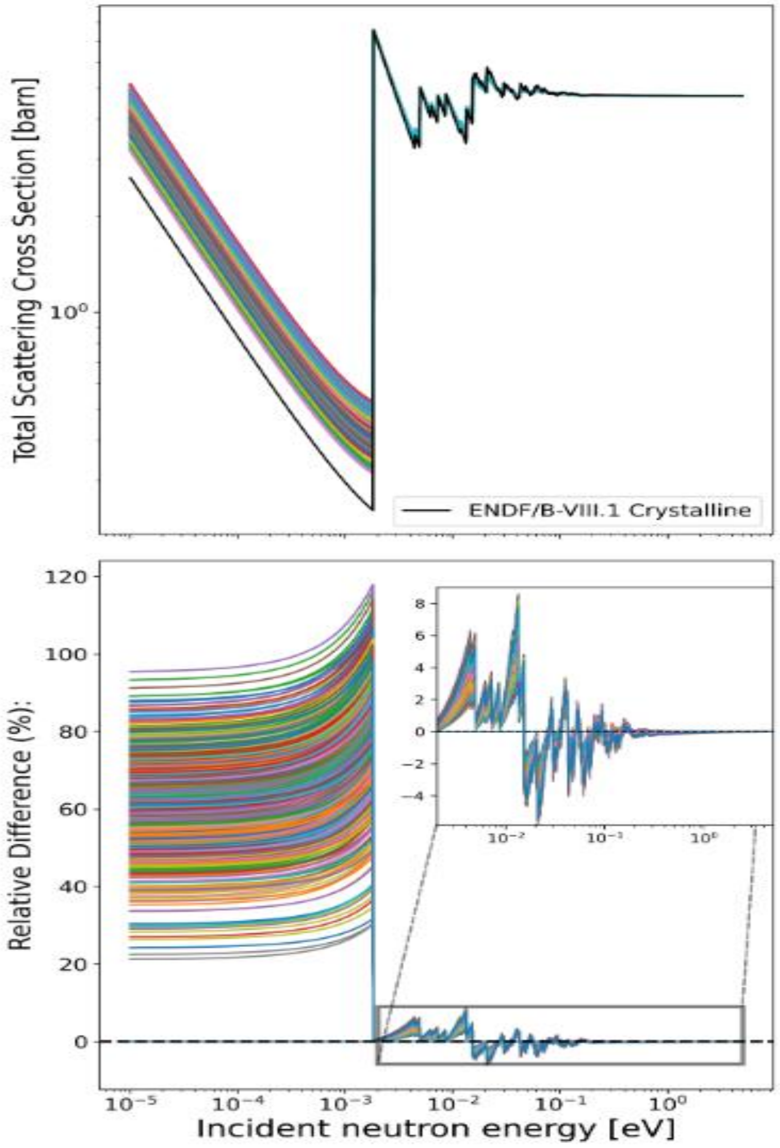
TARA: GRAPHITE TSL | SAMPLING 2

Restricted sampling using the Crystalline graphite TSL available in ENDF/B-VIII.1 (peak position perturbation)



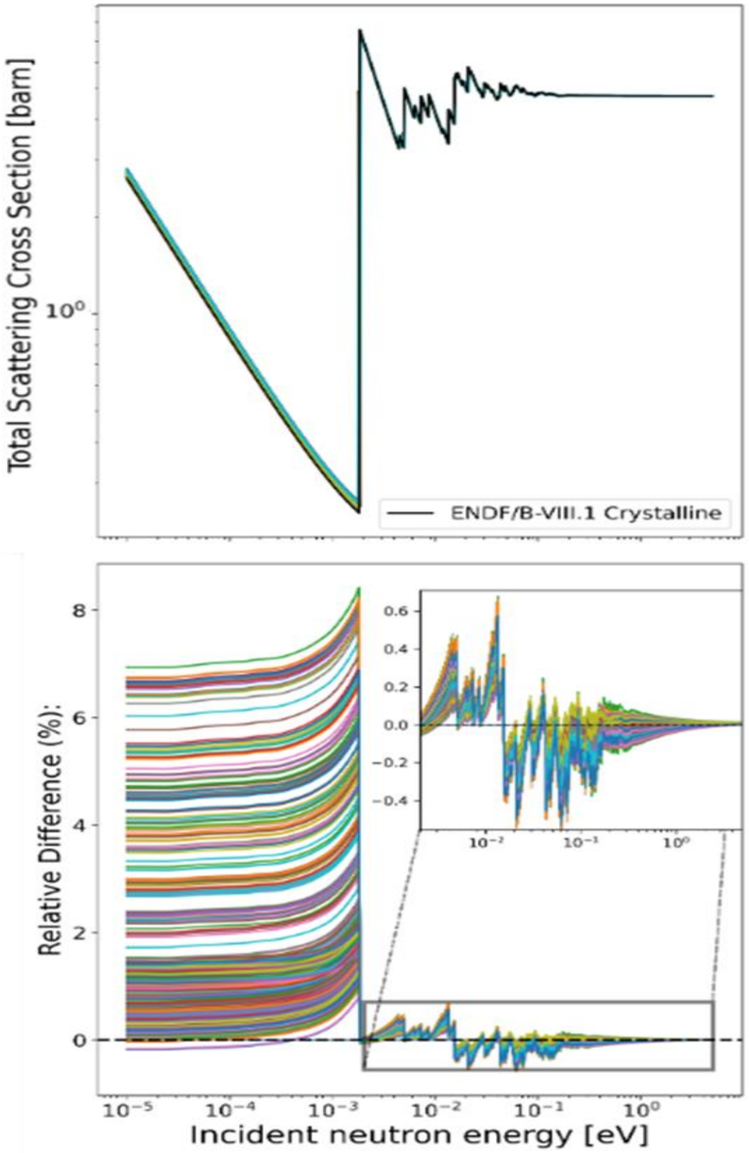


TARA: GRAPHITE TSL | WHAT DO WE LEARN ?



- Estimation of TSL uncertainty is very sensitive to the way we carry out sampling.
- In this example, graphite shows two very different trend (spread of 8% vs 120% in the cross section variation) for the same TSL.
- TARA takes these into account and help march towards TSL correlation and covariance matrix development.

Procedural Choices Determine Thermal Scattering Law Uncertainties



CONCLUSIONS | WHAT'S NEXT…

- Two sampling technique gives completely different results. Indicates a controlled sampling for TSL necessary rather than random (blind) sampling.
- We will test the impact of these sampled Graphite TSL on benchmarks sensitive to Graphite.
- So far TARA can sample:
  - Light Water
  - Graphite (this work)
  - Polyethylene (in progress)
- Elaborate the sampling methodology for more moderator material and the use of NCrystal.
- Release a preliminary version of TARA to be able to have quick user feedbacks.