

INTERCOMPARISON OF NUCLEAR DATA PROCESSING

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THE FUNDAMENTAL QUESTION

The Reality

- Neutronics simulations rely on evaluated nuclear data (ENDF format)
- ENDF files cannot be used directly by Monte Carlo codes
- Must be "**processed**" into usable formats (ACE files)

Nuclear Data Processing

A Hidden Variable in Criticality Safety

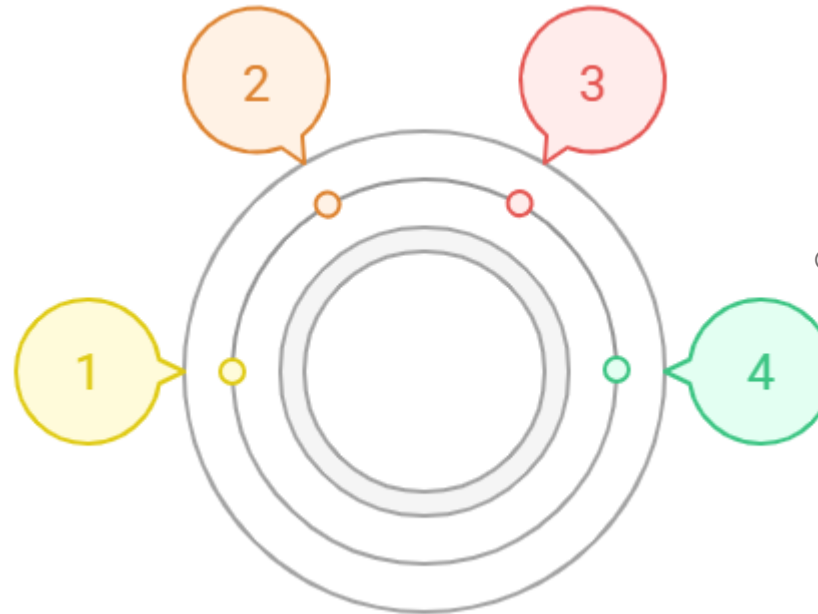
The Problem

Multiple nuclear data processing codes (using somewhat different algorithms):

- NJOY (LANL, US)
- FUDGE (LLNL, US)
- GAIA (ASNR, France)
- AMPX (ORNL, US)

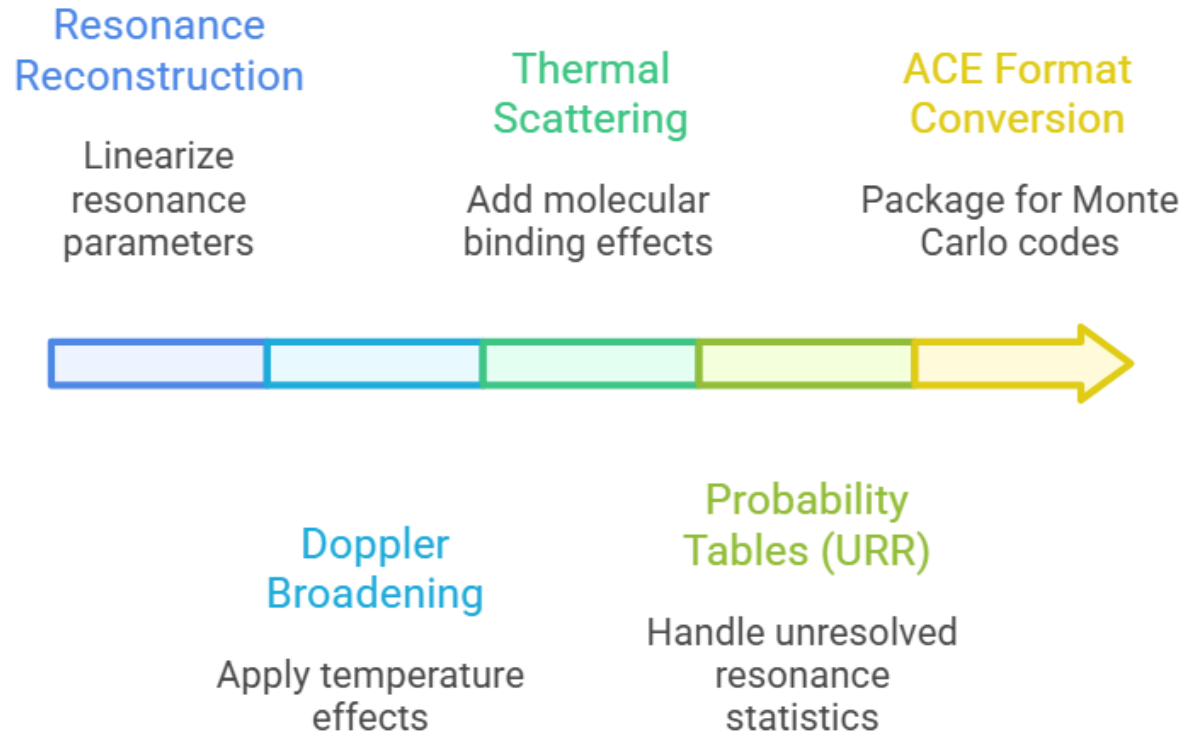
The Question

- Do these processing differences matter for criticality safety?
- Or do they all produce equivalent results?



WHAT ACTUALLY HAPPENS DURING PROCESSING


Five Critical Processing Steps:




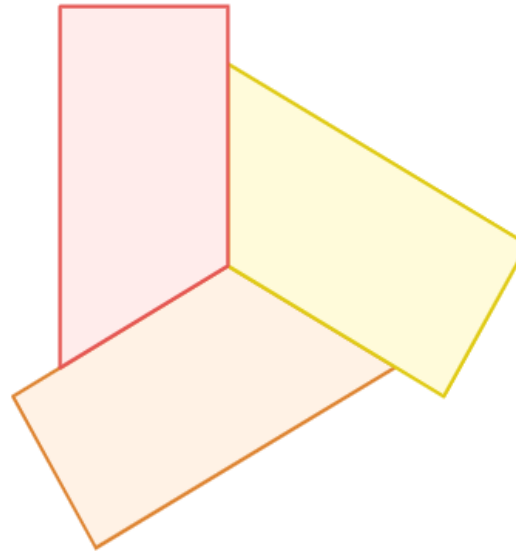
Even small algorithmic differences can propagate through all five steps


WHAT ACTUALLY HAPPENS DURING PROCESSING

Five Critical Processing Steps:

FUDGE 
Python-based
code allowing
flexible
processing order.

GAIA 
Integrated
workflow where
DOP combines
steps 1 and 2.

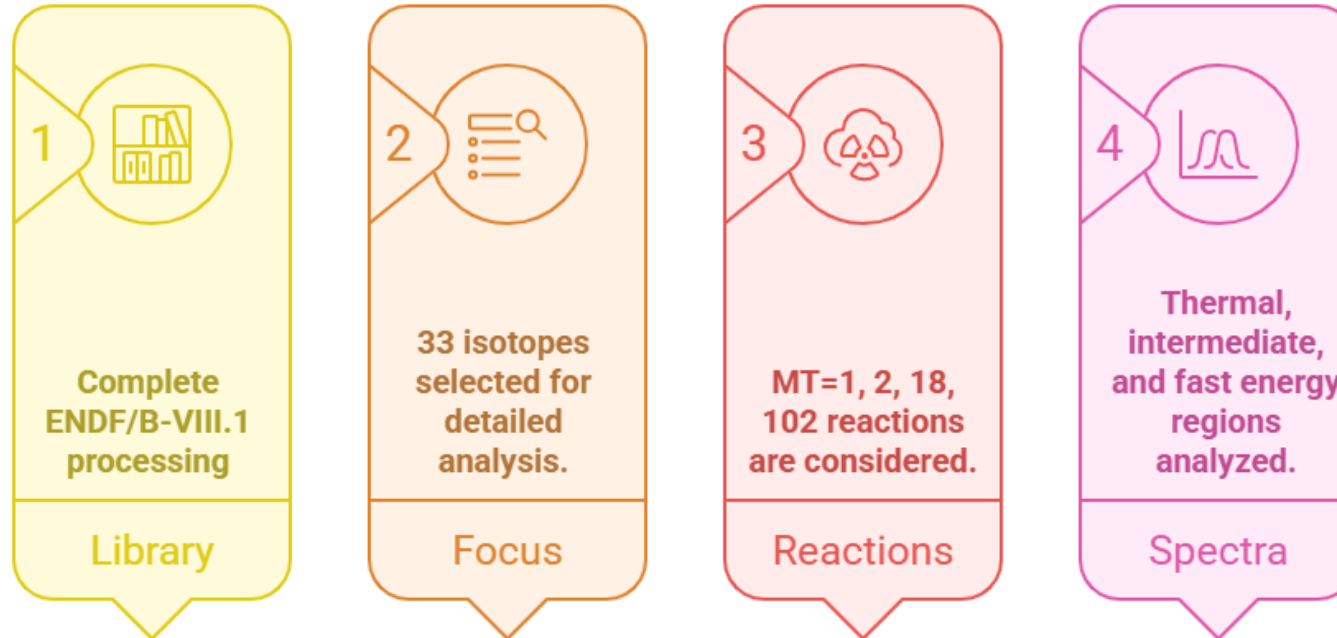


 **NJOY**
Modular Fortran
code using
sequential
processing.

*Even small algorithmic
differences can propagate
through all five steps*

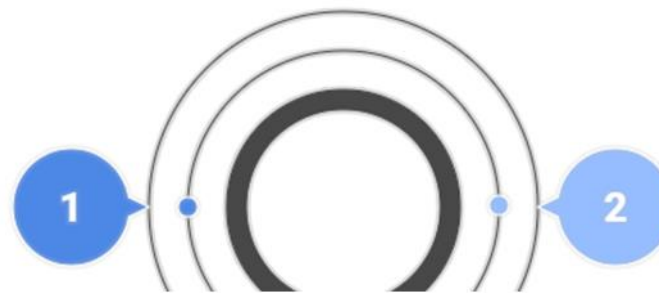
OUR INVESTIGATION STRATEGY

Quantify how processing methodology affects neutronics simulations



Cross Section Differences

- Direct ACE/PENDF file comparison
- Energy-dependent relative differences
- Identify where codes disagree

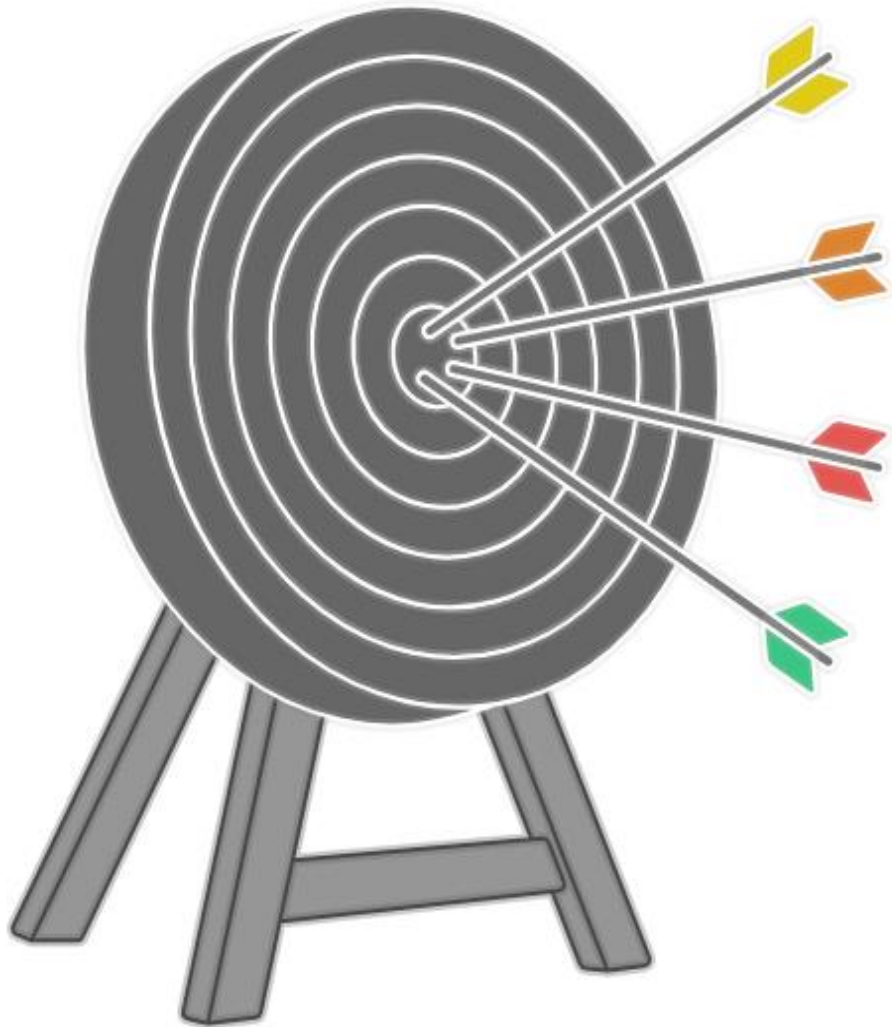


Two-Level Analysis

Impact on Criticality

- ICSBEP benchmark calculations
- k_{eff} variations between codes
- Correlation: cross sections → reactivity effects

METHODOLOGICAL RIGOR



Phase 1: Baseline Establishment (This Work)

- ✓ All codes use default (user-defined) processing parameters
- ✓ Same ENDF/B-VIII.1 source data
- ✓ Identical temperature grids

Phase 2: Parameter Sensitivity (Planned)

- Systematic variation of reconstruction tolerances
 - Different thermal scattering treatments
- Variation of several other processing parameters

Quantitative Metrics

- $\Delta\sigma/\sigma$
- Energy-integrated differences by region
 - Statistical distribution analysis

Validation Approach

- CALINS tool → sensitive benchmark selection
- 5 benchmarks per isotope covering different neutron spectra
 - Correlate cross sections with k_{eff} variations

ANALYSIS WORKFLOW

Strategic Selection Covering Key Nuclear Applications

Actinides (12):

- ❖ Uranium: ^{234}U , ^{235}U , ^{236}U , ^{238}U
- ❖ Plutonium: ^{238}Pu , ^{239}Pu , ^{240}Pu , ^{241}Pu , ^{242}Pu
- ❖ Minor Actinides: ^{237}Np , ^{241}Am , ^{243}Am

Fission Products (15):

- ❖ Neutron Poisons: ^{103}Rh , ^{133}Cs , ^{149}Sm , ^{152}Sm , ^{155}Gd
- ❖ Other FP: ^{95}Mo , ^{99}Tc , ^{101}Ru , ^{109}Ag , ^{143}Nd , ^{145}Nd , ^{147}Sm , ^{150}Sm , ^{151}Sm , ^{153}Eu

Structural Materials (6):

- ❖ Iron: ^{54}Fe , ^{56}Fe , ^{57}Fe , ^{58}Fe
- ❖ Copper: ^{63}Cu , ^{65}Cu

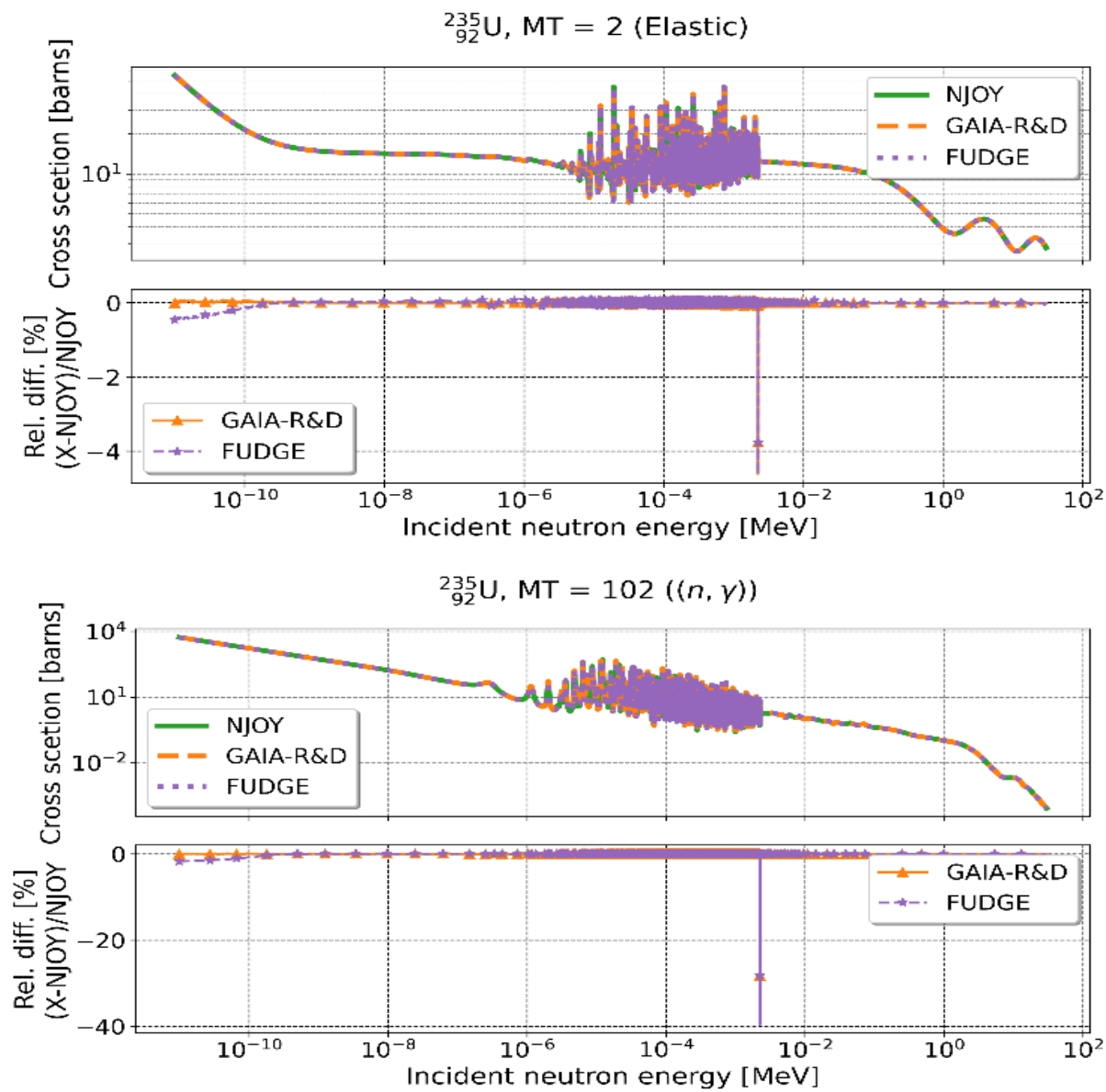
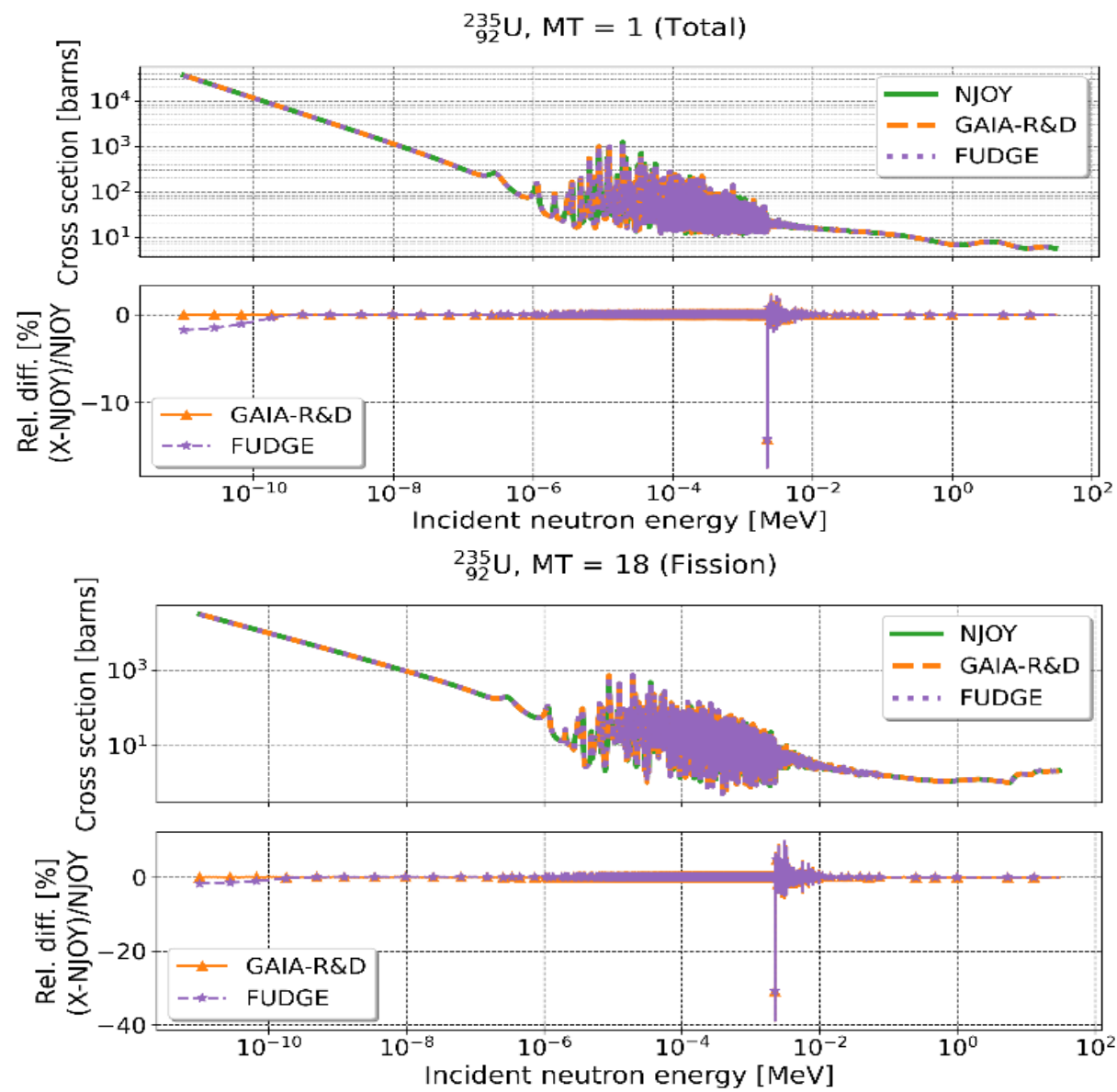
Selection Rationale:

- Criticality safety relevance across all spectra
- Diverse nuclear properties (fissile, fertile, absorbers)
- Representative of reactor fuel and structural compositions

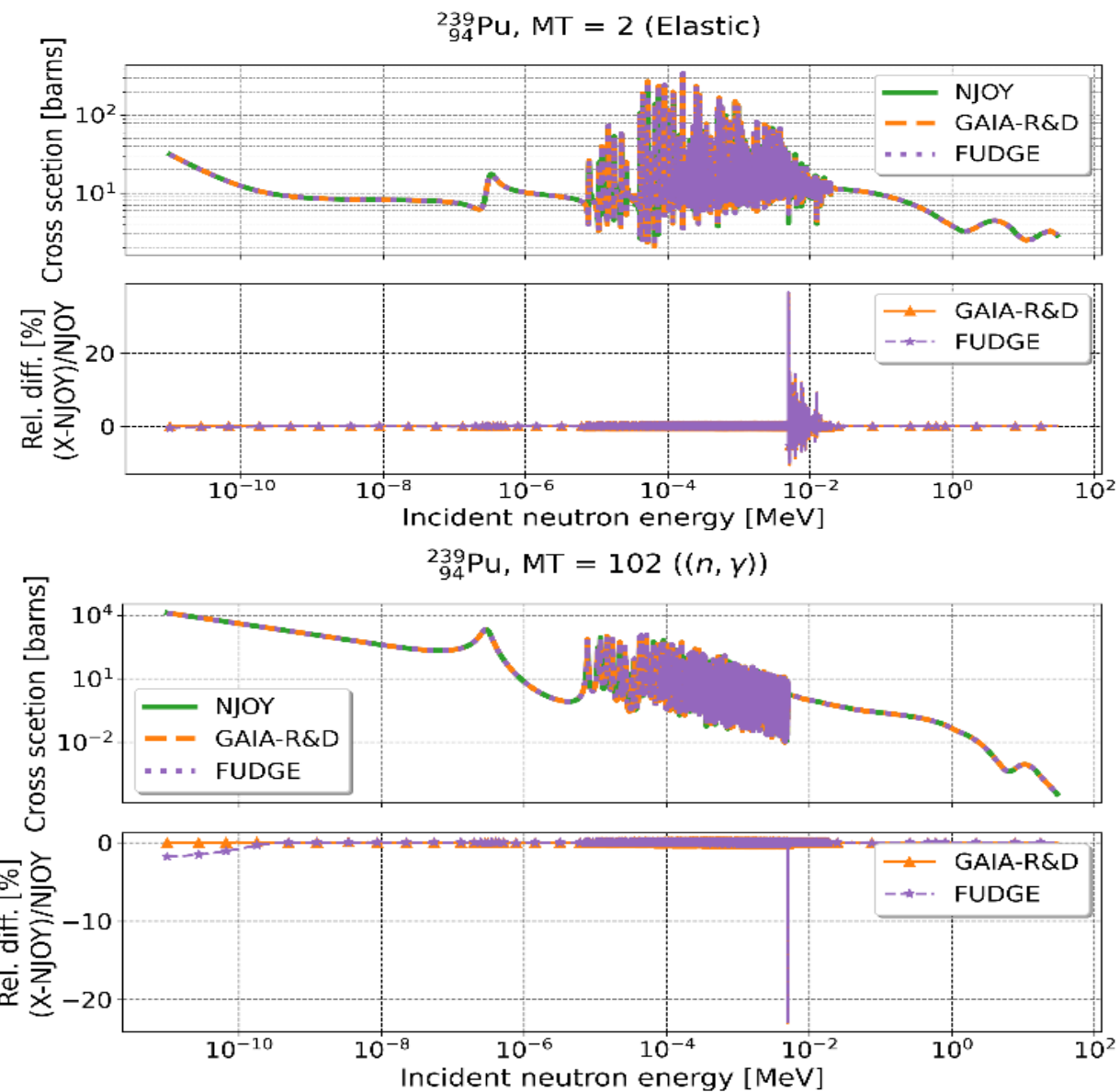
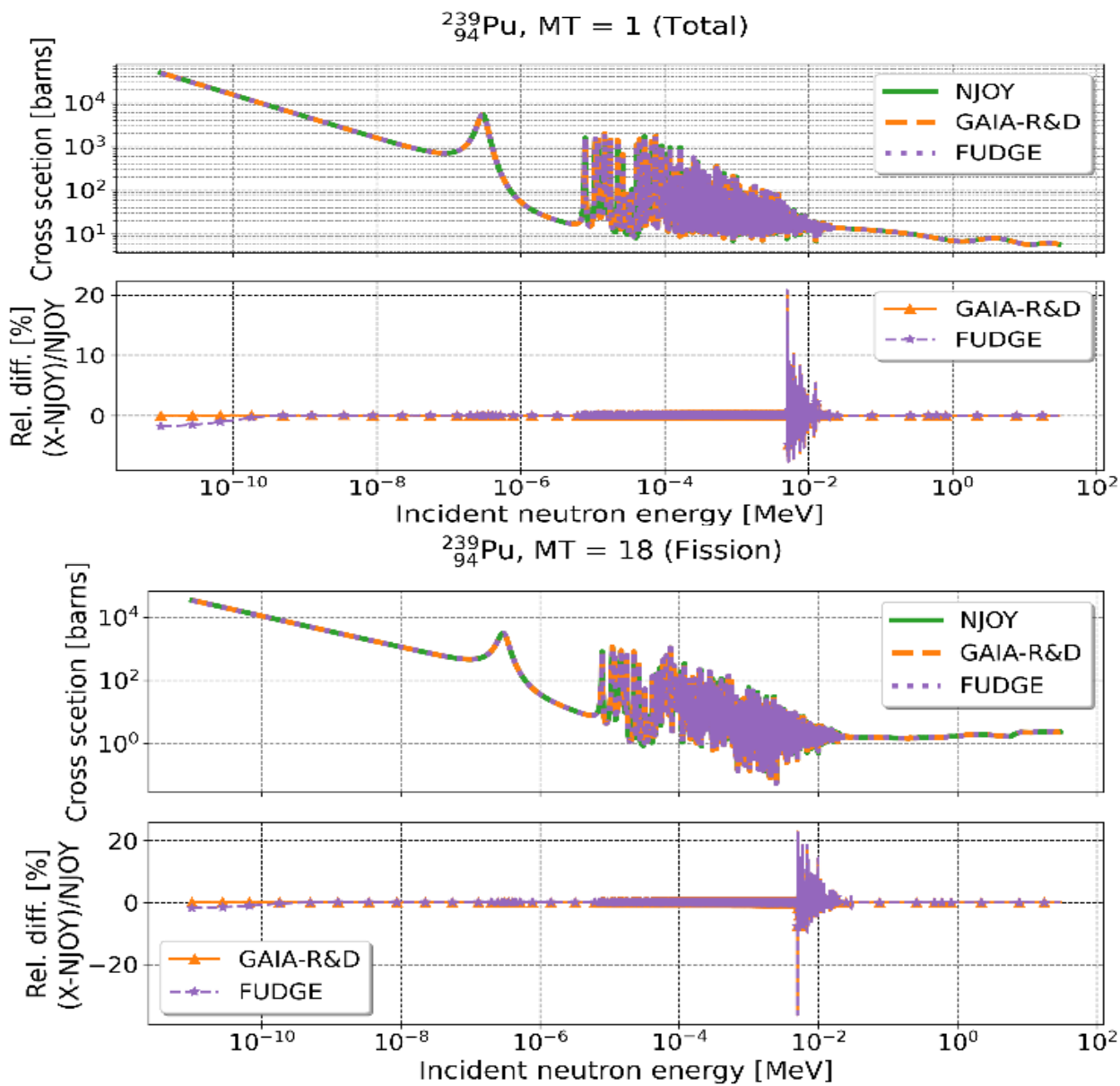
Study Approach:

- ❖ **Phase 1 (This Presentation):** Default parameters used for FUDGE, NJOY, and GAIA → Establishes baseline comparison → Identifies inherent code methodology differences
- ❖ **Phase 2 (Planned):** Systematic parameter variation study → Quantifies parameter sensitivity → Separates parameter effects from methodology differences → *AMPX processing to be included in future phase*

PRELIMINARY RESULTS - CROSS SECTIONS: U235

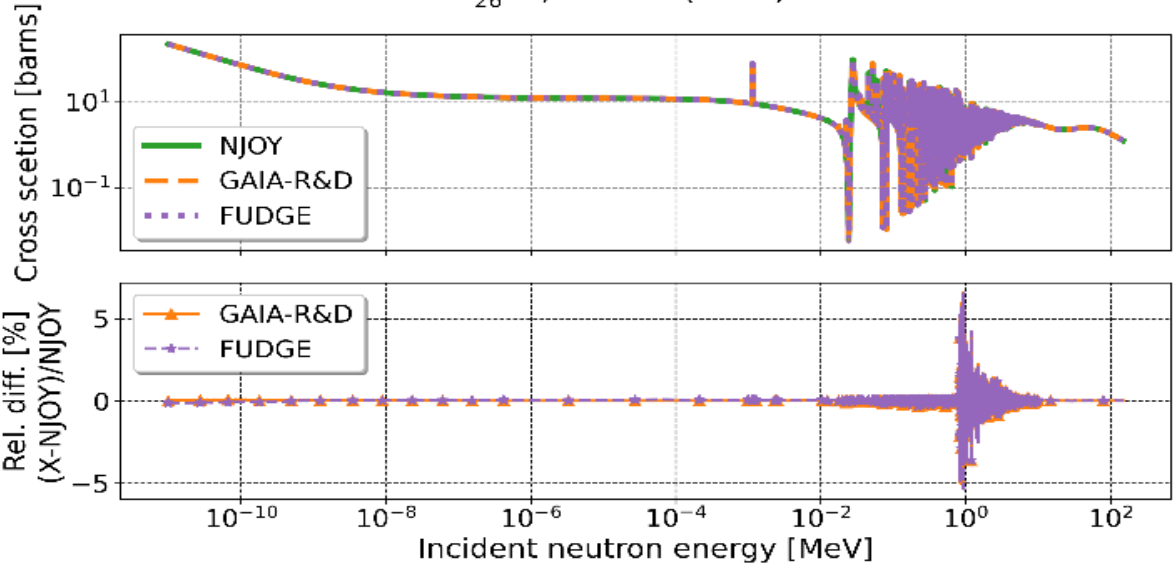


PRELIMINARY RESULTS - CROSS SECTIONS: PU239

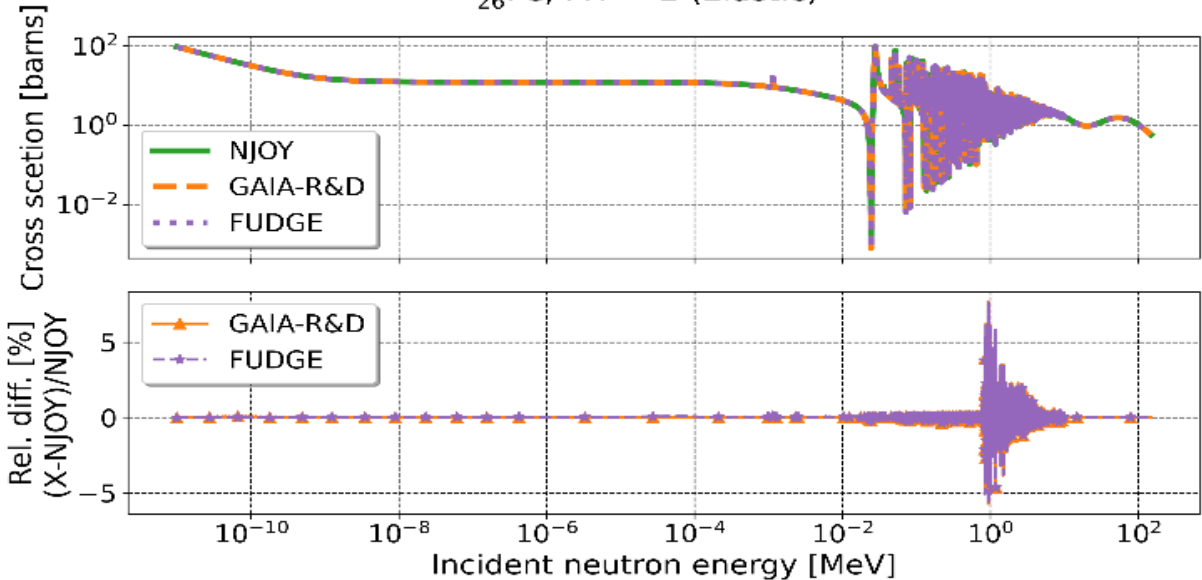


PRELIMINARY RESULTS - CROSS SECTIONS: FE56

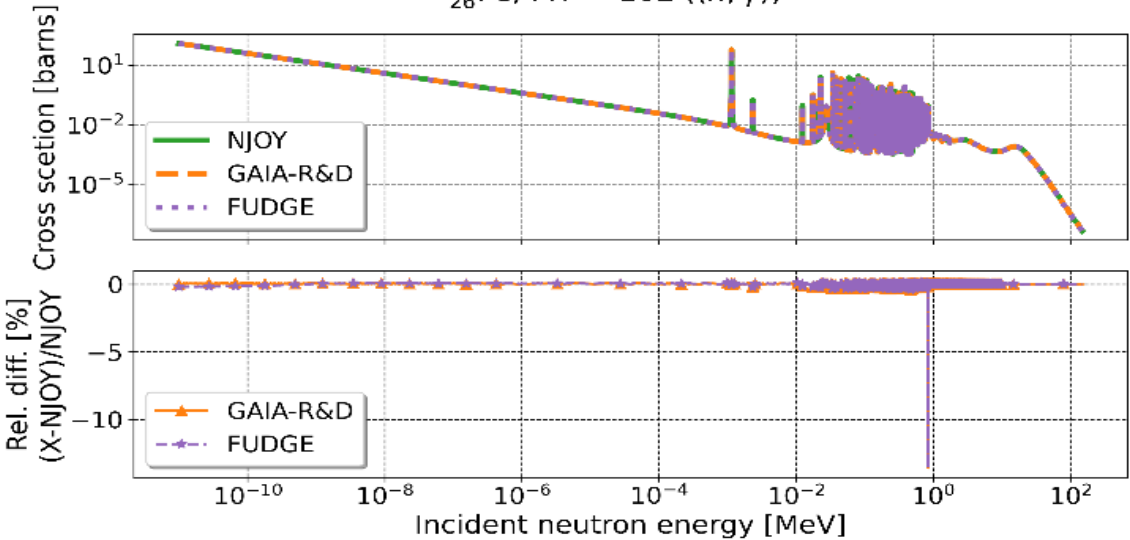
$^{56}_{26}\text{Fe}$, MT = 1 (Total)



$^{56}_{26}\text{Fe}$, MT = 2 (Elastic)



$^{56}_{26}\text{Fe}$, MT = 102 ((n, γ))



BENCHMARK IMPACT

DICE Database: 4,259 ICSBEP Benchmarks

Sensitivity data in .sdf format

Sensitivity Criterion

$$\left| \sum_{i=X}^Y S_i \right| > \theta$$

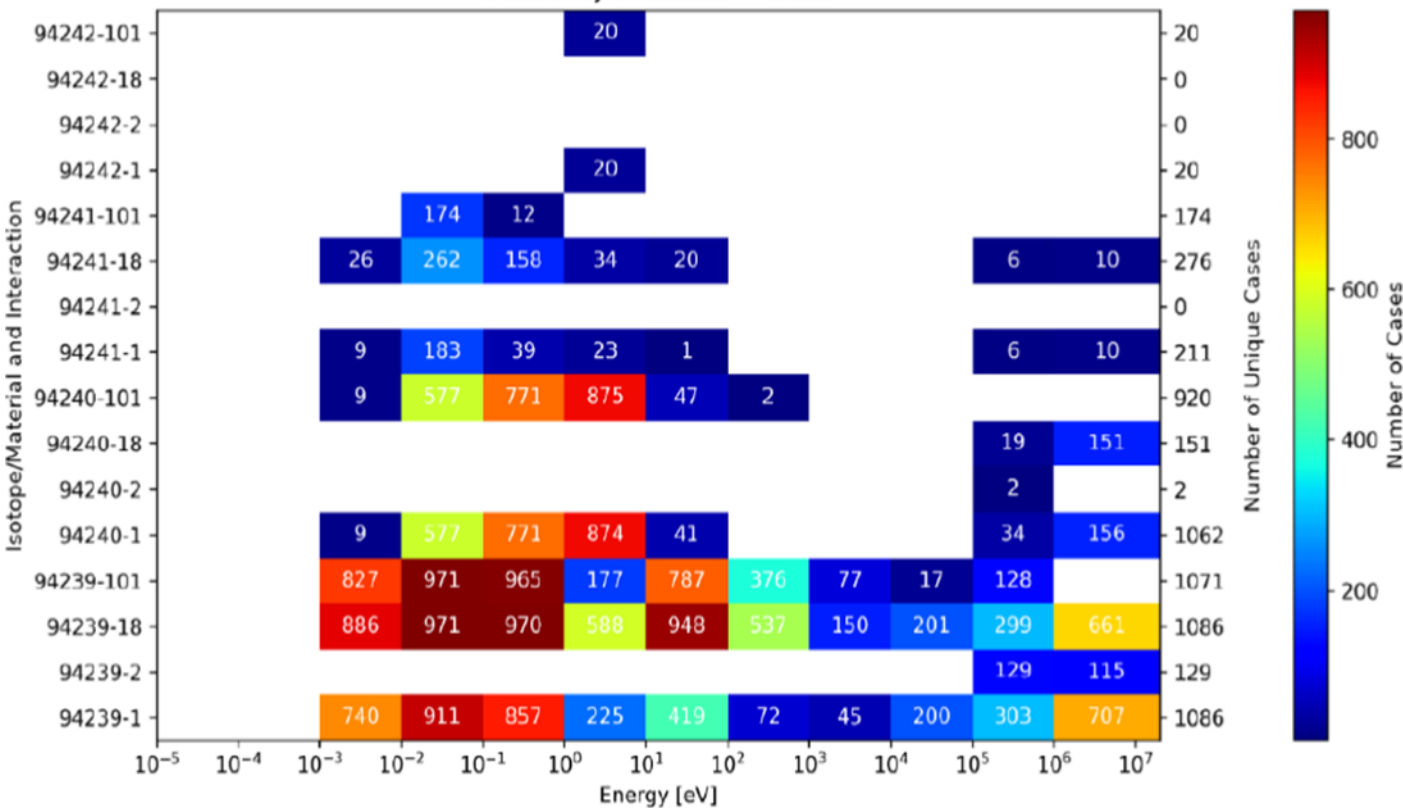
θ = user-defined threshold

Three Spectral Regions

Thermal: 1e-5 eV → 0.605 eV
Intermediate: 0.605 eV → 100 keV
Fast: 100 keV → 20 MeV

Selected Benchmarks

5 benchmarks per isotope covering all spectra
165 total benchmarks for 33 isotopes



Sensitivity heatmap of ICSBEP benchmarks for the total, capture, elastic, and fission for Pu

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Sensitivity data in .sdf format

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NJOY GAIA Delta
Thermal energy region

1	PU-SOL-THERM-012-004	1.00219	1.00154	-64
2	PU-SOL-THERM-012-003	1.00093	1.00112	20
3	PU-SOL-THERM-012-002	1.00018	1.00005	-12

Intermediate energy region

1	MIX-MET-INTER-004-001	0.97992	0.97973	-18
2	MIX-MET-INTER-003-001	0.97053	0.96981	-71
3	PU-MET-INTER-002-001	1.00391	1.00375	-15
4	MIX-MISC-MIXED-001-004	1.00654	1.00666	13

Fast energy region

1	PU-MET-FAST-022-001	0.99784	0.99824	41
2	PU-MET-FAST-001-001	1.00100	1.00040	-59
3	PU-MET-FAST-025-001	0.99977	0.99984	8
4	PU-MET-FAST-035-001	0.99714	0.99708	-5
5	PU-MET-FAST-040-001	0.99362	0.99341	-20

**A preliminary result of GAIA and NJOY processing
effect on benchmarks sensitive to Pu239**

PRELIMINARY CONCLUSIONS

Status

- This is a kick-off study demonstrating feasibility.
- Robust, large-scale work is needed next.

Initial Findings

- Processing codes produce generally good agreement (~1% typical)
- Local differences in certain energy regions (resonances, URR)
- Differences arise from algorithmic choices, not errors



Key Insight

- Cross section variations are quantifiable
- But their impact on criticality safety needs comprehensive investigation

Methodology Established

- Systematic framework for comparing processing codes
- Automated workflows and analysis tools Quasi-operational

Process ENDF/B-VIII.1 library using major codes

- FUDGE
- NJOY
- GAIA
- AMPX
- Any other ?

Develop a common standard

- All isotopes, all temperatures, all reaction channels
- Standardized comparison methodology

Why This Matters

Current work demonstrates how to compare an entire nuclear data library (processing effect) needed for meaningful criticality safety conclusions.

The Real Work Begins Now

Comprehensive
Baseline Processing
Campaign



International Collaboration

We envision working on this exercise with participants from: ORNL, LLNL, LANL, NNL

THE BROADER VISION

Launch Full-Scale Campaign (FY 2026)

- ❖ Coordinate with ORNL, LLNL, LANL, NNL
- ❖ Collect/share processed nuclear data libraries
- ❖ Establish common quality metrics

Finalize Current Study

- ❖ Carry out ICSBEP benchmark calculations with NJOY, GAIA, FUDGE and AMPX with baseline parameters for all 33 isotopes

Systematic Parameter Studies

- ❖ Processing parameter sensitivity
- ❖ Temperature effects
- ❖ Thermal scattering treatment variations

Our Ask to Collaborators:

- ❖ Active participation in processing efforts
- ❖ Joint analysis of results

Timeline:

- ❖ Ready to start working robustly—we need your involvement to make it comprehensive and credible.
- ❖ This presentation demonstrates the methodology and invites collaboration for the real work ahead.

