

Release of ENDF/B-VII.1-based Continuous-Energy Neutron Cross-Section Data Tables for MCNP

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Introduction

ENDF/B-VII.1

Evaluated Nuclear Data File Version 7.1

- Released December 2011
- Neutron sublibrary:
 - 423 evaluations, 32 new in ENDF/B-VII.1
 - Elemental evaluations for V and Zn became isotopic evaluations:
 ^{50}V , ^{51}V and ^{64}Zn , ^{65}Zn , ^{66}Zn , ^{67}Zn , ^{68}Zn
 - 10 excited-state evaluations, 413 ground-state evaluations

ENDF71x

ENDF/B-VII.1-based ACE data tables

- 423 evaluations
- 7 temperatures
 - 293.6 K
 - 600 K
 - 900 K
 - 1200 K
 - 2500 K
 - 0.1 K
 - 250 K
- 2 modifications from ENDF/B-VII.1
 - ^{56}Fe , σ_s
 - ^{61}Ni , σ_s
- Processed using NJOY Version 99.393

Modifications to ENDF/B-VII.1

^{56}Fe

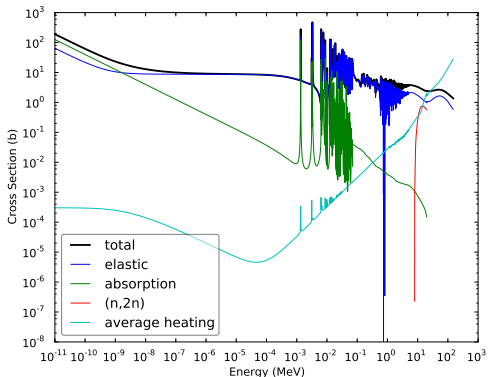
- $0.0 \text{ b } \sigma_s \text{ (MT=2)}$
- $E = 1.1971 \text{ MeV}$

^{61}Ni

- $0.0 \text{ b } \sigma_s \text{ (MT=2)}$
- $E = 0.7429251 - 0.743962 \text{ MeV}$
- $E = 0.8184120 \text{ MeV}$

σ_s Changed to $1 \times 10^{-6} \text{ b}$

^{61}Ni



Modifications to ENDF/B-VII.1

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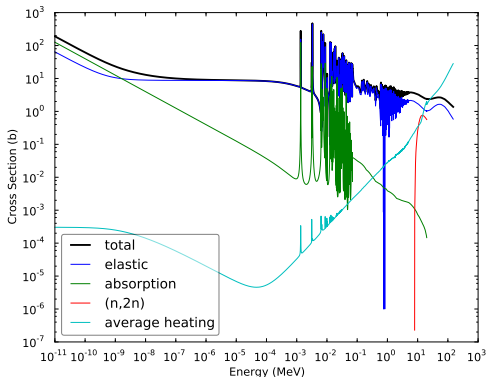
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Verification of ENDF71x

checkace

- Appropriate threshold representation
- Negative PDFs
- Unphysical secondary particle energies
- Heating balance problems—negative heating values
- Partial xs summing to total

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Visual inspection of cross sections

- Identify *gross* errors
 - σ_t , MT=1
 - σ_a , MT=102
 - σ_{es} , MT=2
 - $\sigma_{(n,2n)}$, MT=16
 - average heating number
kerma* σ_t

Verification—Negative PDFs



- Originates in ENDF/B-VII.1 evaluation
- MT=91, (n, n') — n' in the continuum
- Negative PDF values set to 0.0 in ENDF71x ACE data tables

Verification—Energy Balance

Negative Heating Values

- 41 evaluations
- Problems when performing energy deposition or kerma calculations
- *Probably* not a major impact on calculations
- These evaluations (and others) have been identified by Bob MacFarlane as having problems with energy balance.
<http://t2.lanl.gov/data/endl/eбалVII.1/summary.html>
- Evaluations need to be improved in future ENDF/B-VII.1 releases

Verification—Unresolved Resonance Region

Sum of partial cross sections don't add to the total in URR

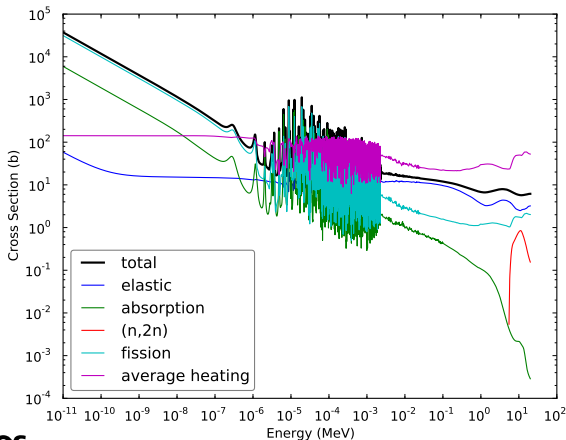
- Most errors are close to round-off
- 15 evaluations—listed in paper/documentation
- NJOY PURR module not run for these evaluations
 - Average cross sections are used instead of an unresolved resonance representation

Visual Inspection of Major Cross Sections

- Visual inspection
 1. σ_t , MT=1
 2. σ_a , MT=102
 3. σ_{es} , MT=2
 4. $\sigma_{(n,2n)}$, MT=16
 5. average heating number
kerma* σ_t

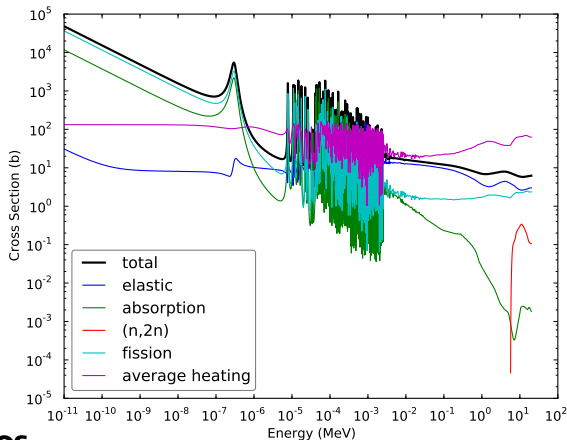
Visual Inspection of Major Cross Sections

^{235}U



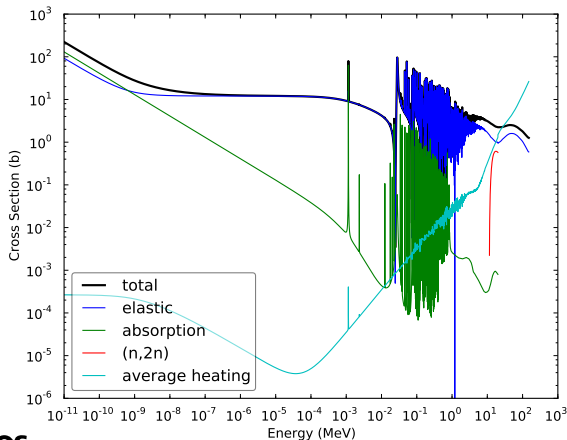
Visual Inspection of Major Cross Sections

^{239}Pu



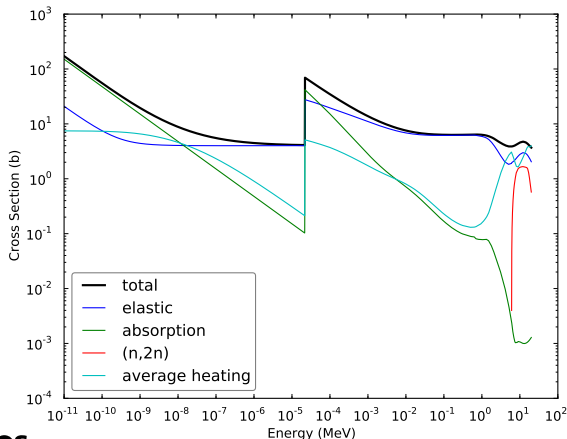
Visual Inspection of Major Cross Sections

^{56}Fe



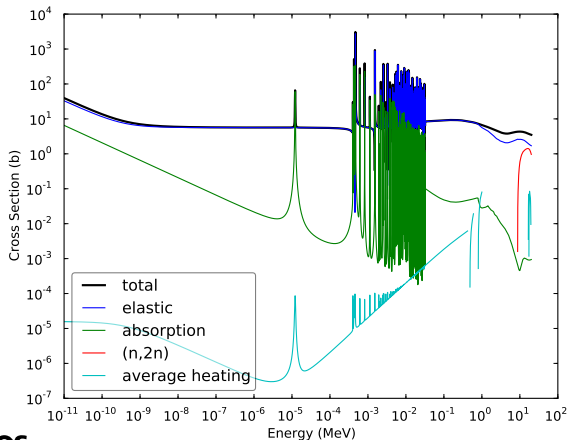
Visual Inspection of Major Cross Sections

^{123}Sn



Visual Inspection of Major Cross Sections

^{98}Mo



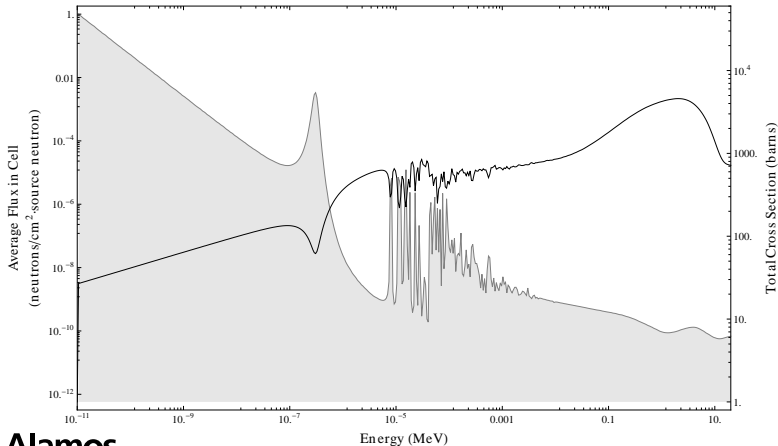
Mechanical Testing

- 4 cm sphere
- One isotope
- Nominal density for element
- $1 \times 10^{-11} \text{ MeV} \leq E \leq 20 \text{ MeV}$
- Three energy distributions:
 1. Uniform
 2. Watt fission spectrum
 3. Room temperature Maxwellian
- mode n p
- 1×10^9 histories
- Tallies:
 - F1 Outer surface current
 - F2 Outer surface flux
 - F4 Volume flux
- 500 logarithmically-spaced energy bins

Mechanical Testing

Results

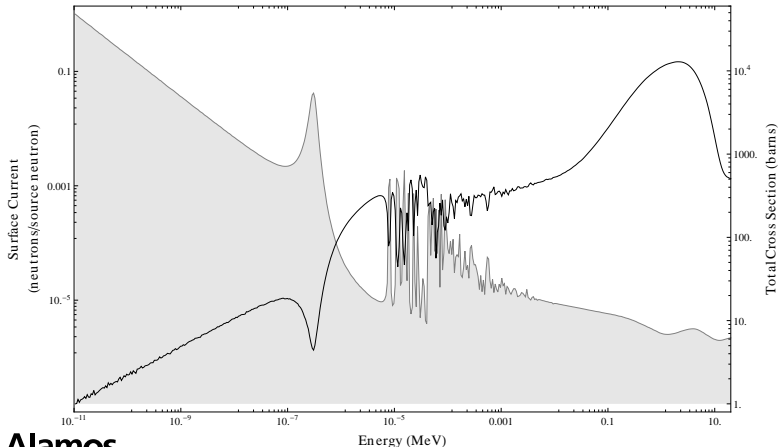
Average Flux of Neutrons Within the Pu-239 Sphere



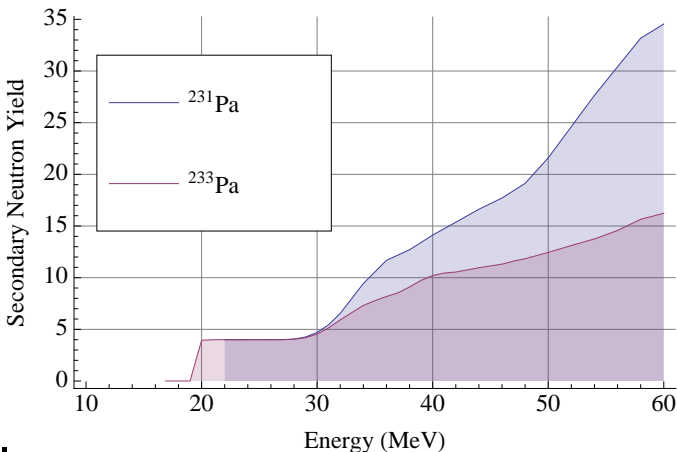
Mechanical Testing

Results

Surface Current of Neutrons Leaving the Pu-239 Sphere



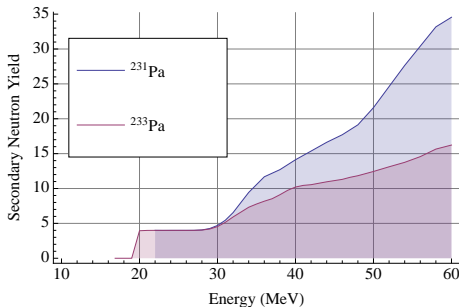
Mechanical Testing—(Too) Many Secondaries



Mechanical Testing—(Too) Many Secondaries

- MT=5, ($n, *$) $^{231,233}\text{Pa}$
- < 12 secondaries assumed
- If ≥ 12 secondaries:
 - Array bounds exceeded
 - Unknown quantities changed
 - (very) Negative energies

This has *not* been fixed in MCNP



Validation Testing

- 423 evaluations
- 7 temperatures
- 3 source energy distributions
- MCNP5 *and* MCNP6
- 1×10^9 histories each
- 715 critical benchmarks,
13,702 CPU hours

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Most heavily verified and validated ACE data library
ever released with MCNP

ZAIDs in ENDF71x

ZA Suffix	SZA eXtension	Temperature
80c	710nc	293.6 K
81c	711nc	600 K
82c	712nc	900 K
83c	713nc	1200 K
84c	714nc	2500 K
85c	715nc	0.1 K
86c	716nc	250 K

$$92235.80c = 92235.710nc$$

Listing of Available ACE Data Tables

(formerly*known as Appendix G of the MCNP Manual)

Jeremy Lloyd Conlin, D. Kent Parsons, Steven J. Gardiner, Mark Gray, A. C. Kahler, M. Beth Lee, and Morgan C. White

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Conclusion

- ENDF/B-VII.1—released December 2011
 - 423 evaluations, 32 new
 - Best neutron cross section data available
- ENDF71x
 - Based on ENDF/B-VII.1—processed with NJOY version 99.393
 - 7 temperatures suitable for reactor and laboratory calculations
 - **Extensive** validation and verification
 - Available with release of MCNP6
- New document listing available ACE data tables—no longer an appendix to MCNP manual