

# LA-UR-13-24077

Approved for public release; distribution is unlimited.

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

Author(s): Conlin, Jeremy Lloyd  
Gardiner, Steven J.  
Parsons, Donald K.  
Kahler, Albert C. III  
Lee, Mary Beth  
White, Morgan C.

Intended for: ANS 2013 Annual Meeting, 2013-06-16/2013-06-20 (Atlanta, Georgia, United States)

Issued: 2013-06-04



**Disclaimer:**

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

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

---

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

*Los Alamos National Laboratory*  
PO Box 1663, Los Alamos NM 87544

June 4, 2013

# 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:  
 $^{50}\text{V}$ ,  $^{51}\text{V}$  and  $^{64}\text{Zn}$ ,  $^{65}\text{Zn}$ ,  $^{66}\text{Zn}$ ,  $^{67}\text{Zn}$ ,  $^{68}\text{Zn}$
  - 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
  - $^{56}\text{Fe}$ ,  $\sigma_s$
  - $^{61}\text{Ni}$ ,  $\sigma_s$
- Processed using NJOY Version 99.393

# Modifications to ENDF/B-VII.1

$^{56}\text{Fe}$

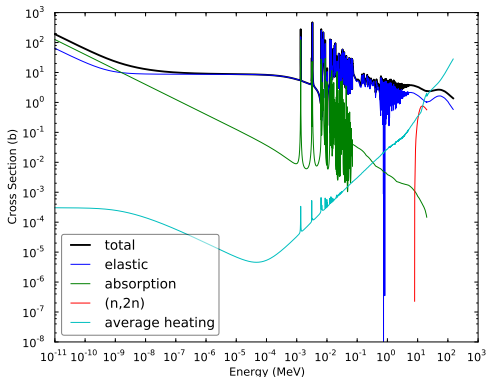
- $0.0 \text{ b } \sigma_s$  (MT=2)
- $E = 1.1971 \text{ MeV}$

$^{61}\text{Ni}$

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

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

$^{61}\text{Ni}$



# Modifications to ENDF/B-VII.1

$^{56}\text{Fe}$

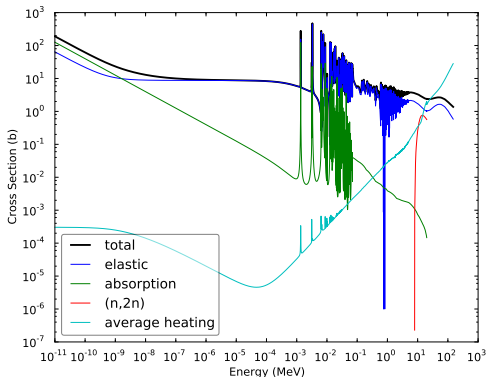
- $0.0 \text{ b } \sigma_s$  (MT=2)
- $E = 1.1971 \text{ MeV}$

$^{61}\text{Ni}$

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

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

$^{61}\text{Ni}$



# Verification of ENDF71x

---

checkace

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

# Verification of ENDF71x

---

## checkace

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

## Visual inspection of cross sections

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



# 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/evalVII.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

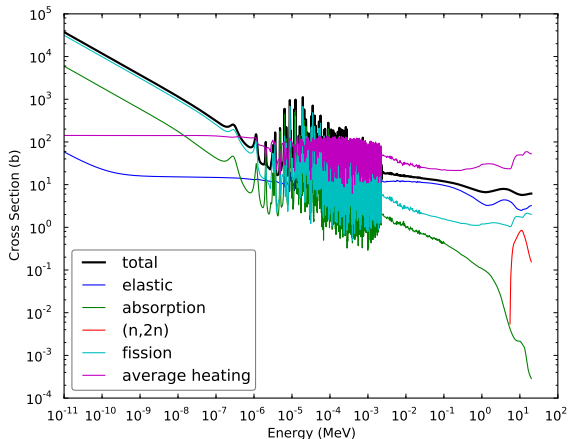
- Most errors are close to round-off
- 15 evaluations—listed in paper/documentation
- NJOY PURR module not run for these evaluations
  - Average cross sections are used instead of an unresolved resonance representation

# Visual Inspection of Major Cross Sections

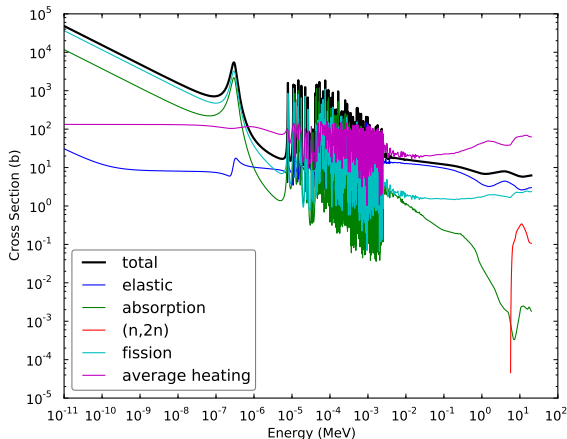
---

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

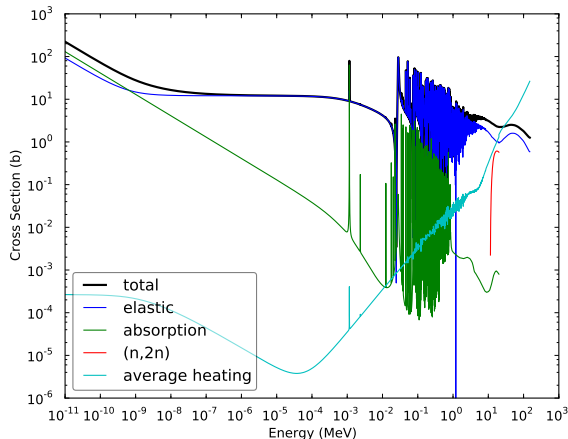
# Visual Inspection of Major Cross Sections



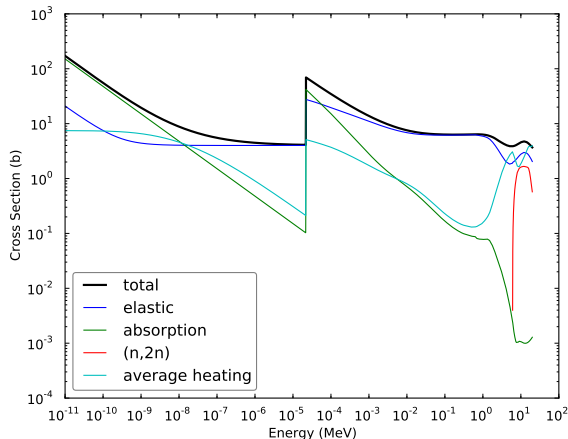
# Visual Inspection of Major Cross Sections



# Visual Inspection of Major Cross Sections

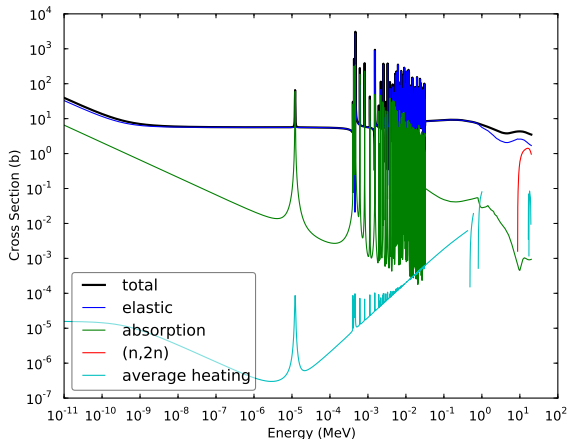


# Visual Inspection of Major Cross Sections





# Visual Inspection of Major Cross Sections



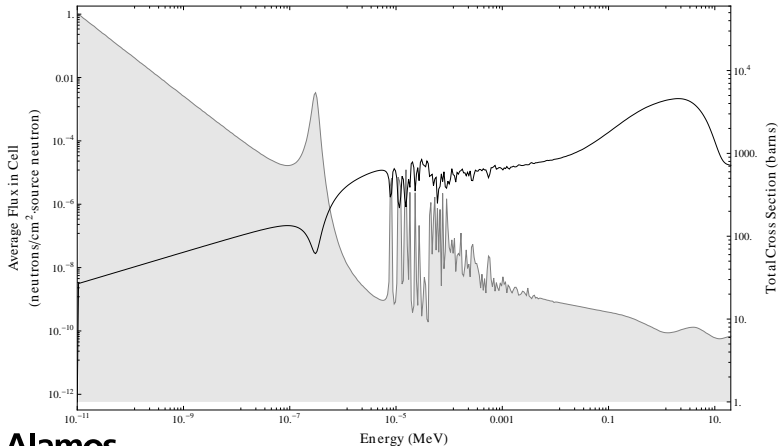
# Mechanical Testing

---

- 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
- $1 \times 10^9$  histories
- Tallies:
  - F1 Outer surface current
  - F2 Outer surface flux
  - F4 Volume flux
- 500 logarithmically-spaced energy bins

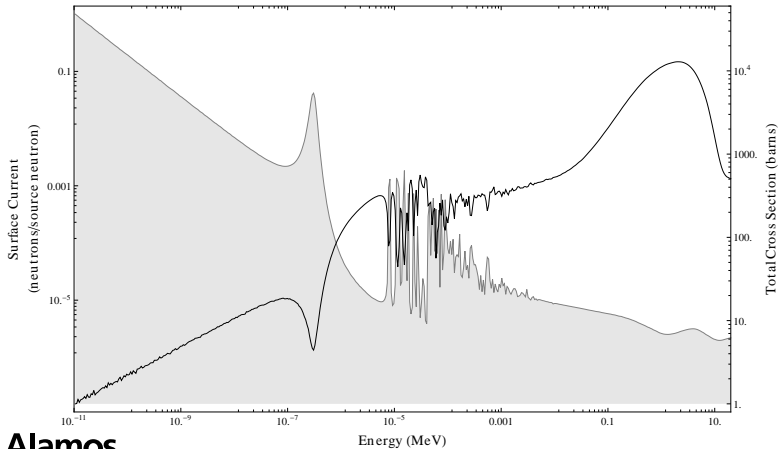
# Mechanical Testing Results

Average Flux of Neutrons Within the Pu-239 Sphere

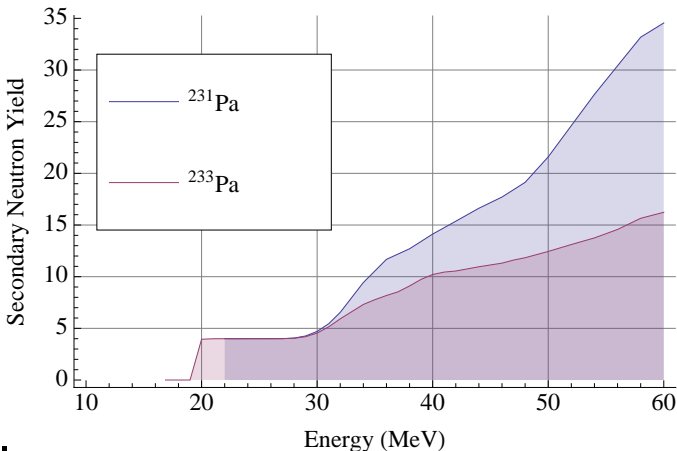


# Mechanical Testing Results

Surface Current of Neutrons Leaving the Pu-239 Sphere



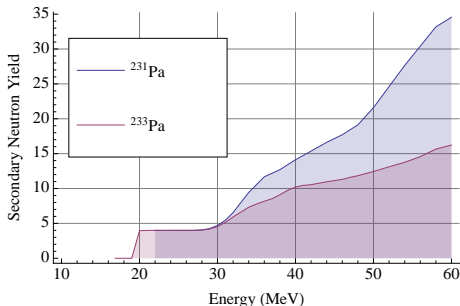
# Mechanical Testing—(Too) Many Secondaries



# Mechanical Testing—(Too) Many Secondaries

- MT=5, ( $n, *$ )  $^{231,233}\text{Pa}$
- < 12 secondaries assumed
- If  $\geq 12$  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
- $1 \times 10^9$  histories each
  
- 715 critical benchmarks,  
13,702 CPU hours

# Validation Testing

---

- 423 evaluations
- 7 temperatures
- 3 source energy distributions
- MCNP5 *and* MCNP6
- $1 \times 10^9$  histories each
- 715 critical benchmarks,  
13,702 CPU hours
- 17,766 MCNP runs
- $> 18 \times 10^{12}$  histories
- 264,841 CPU hours



# Validation Testing

---

- 423 evaluations
- 7 temperatures
- 3 source energy distributions
- MCNP5 *and* MCNP6
- $1 \times 10^9$  histories each
- 715 critical benchmarks,  
13,702 CPU hours
- 17,766 MCNP runs
- $> 18 \times 10^{12}$  histories
- 264,841 CPU hours

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

Nuclear Data Team, XCP-5  
*Los Alamos National Laboratory*

May 10, 2013

# 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