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Title: Data Processing for Criticality Safety at LANL: ENDF/B-VII.1 and Beyond

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Data Processing for Criticality Safety at LANL

ENDF/B-VII.1 and Beyond

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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 evaulations: ^{50}V, ^{51}V and ^{64}Zn, ^{65}Zn, ^{66}Zn, ^{67}Zn, ^{68}Zn
  - 10 excited-state evaluations, 413 ground-state evaluations

Introduction

ENDF/B-VII.1

Evaluated Nuclear Data File Version 7.1

ENDF71x

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

MENDF71x

ENDF/B-VII.1-based `NDI` data tables

Processed using `NJOY` Version 99.393

ENDF71x—ENDF/B-VII.1-based ACE data tables

- 423 evaluations, 32 new
- Best neutron XS data available
- Available with MCNP6 from RSICC
- *Extensive* validation and verification

Temperature	ENDF71x	ENDF70
293.6 K	80c	70c
600 K	81c	71c
900 K	82c	72c
1200 K	83c	73c
2500 K	84c	74c
0.1 K	85c	
250 K	86c	

MENDF71x—ENDF/B-VII.1-based NDI data tables

- 423 evaluations
- Room temperature (293.6 K)
- LANL 618 group structure
  - 250, 133, 70, 30, . . . compatible
- Infinitely dilute (no self-shielding)
- No up-scatter data
- Production-depletion chains
- $S(\alpha, \beta)$ not included
- *Extensive* validation and verification

Verification of ENDF71x and MENDF71x

Verification of ENDF71x and MENDF71x

- $\sum \sigma_x \stackrel{?}{=} \sigma_t \qquad \sum \sigma_{f,x} \stackrel{?}{=} \sigma_f$

Verification of ENDF71x and MENDF71x

- $\sum \sigma_x \stackrel{?}{=} \sigma_t \quad \sum \sigma_{f,x} \stackrel{?}{=} \sigma_f$
- $\int \chi(E) dE \stackrel{?}{=} 1.0, \quad \sum_{i=1}^{G} \chi_i \stackrel{?}{=} 1.0$

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- Unphysical secondary particle energies

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- Negative PDFs

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- Unphysical secondary particle energies
- Negative PDFs

- Visual inspection of cross sections—identify *gross* errors

Warnings and Issues

- 120 evaluations with KERMA problems
  - 41 evaluations with negative heating values
- 38 evaluations with no gamma production data
- ^{153}Eu–negative PDF values for `MT=91`, (n, n')—n' in the continuum
- 53 evaluations with no delayed neutron emission data
- Sum of partials don't add to total in URR for 15 evaluations
- ^{231,233}Pa $>$ 10 secondary neutrons for $E > 34$ MeV
- Some assumptions in `MCNP` are no longer valid with newer data

- Evaluations need to be improved in future releases from NNDC

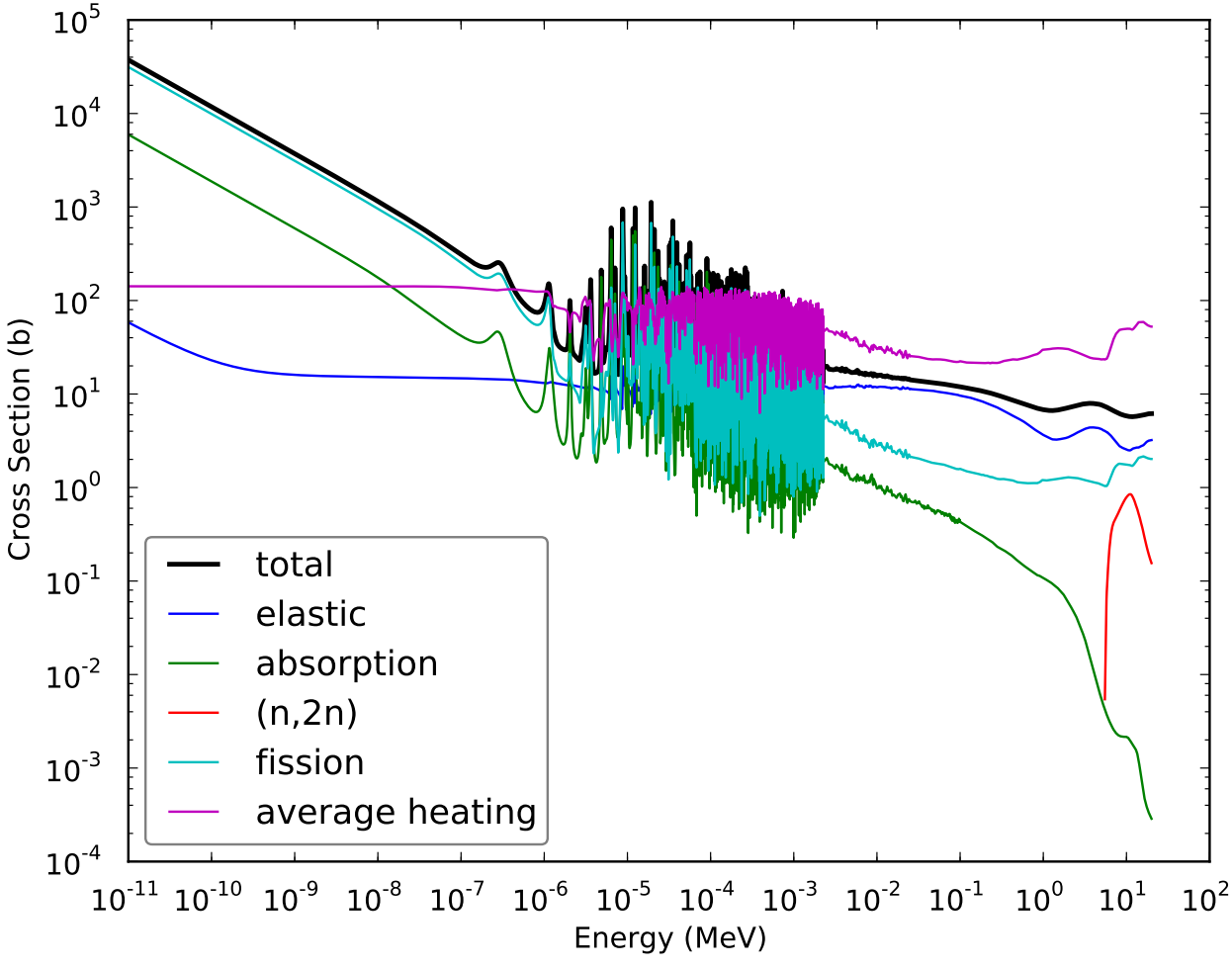
Visual Inspection of Major Cross Sections

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

Visual Inspection of Major Cross Sections

^{235}U

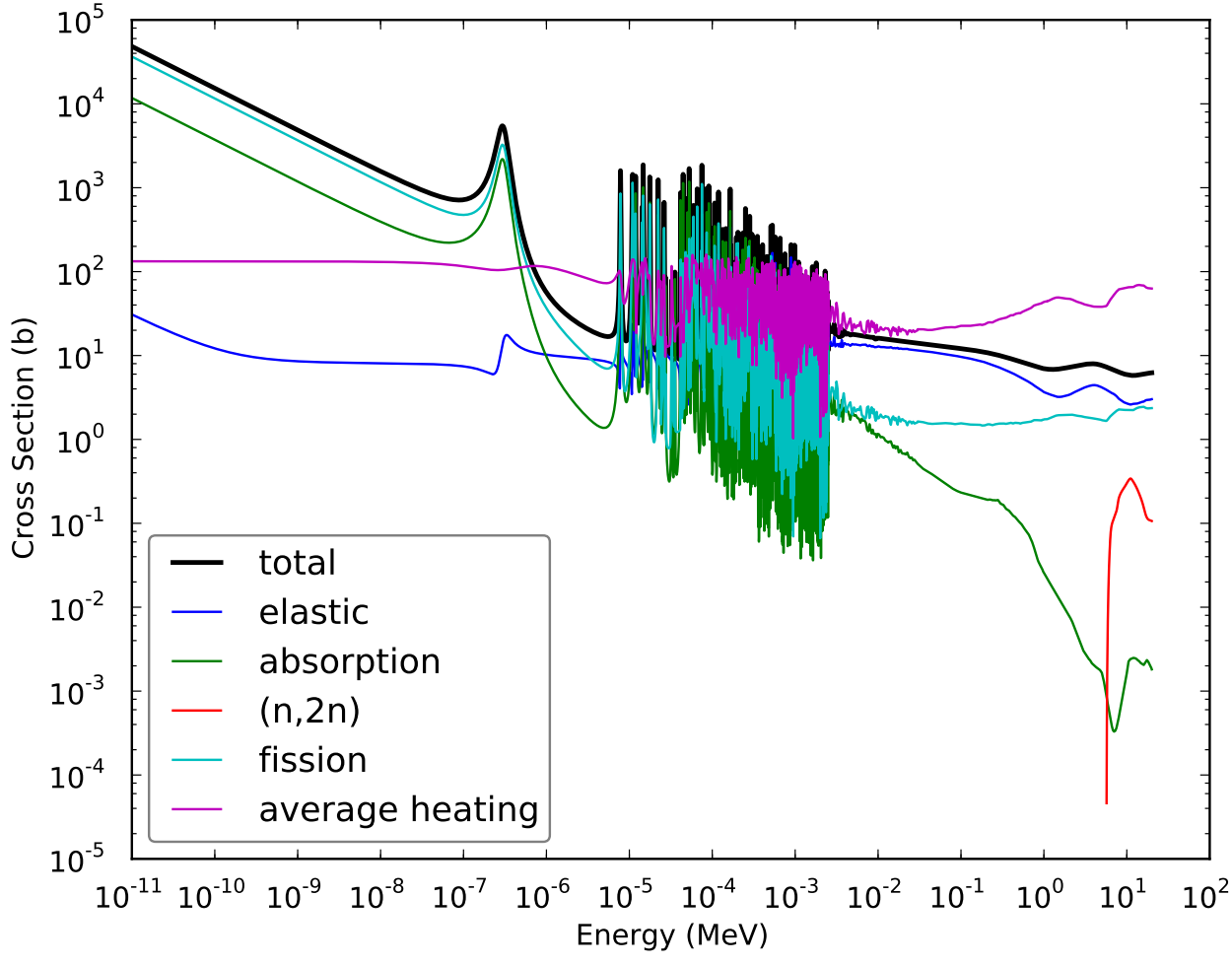
- Visual inspection
  1. σ_t, MT=1
  2. σ_a, MT=102
  3. σ_{es}, MT=2
  4. $\sigma_{(n,2n)}$, MT=16
  5. kerma*σ_t



Visual Inspection of Major Cross Sections

^{239}Pu

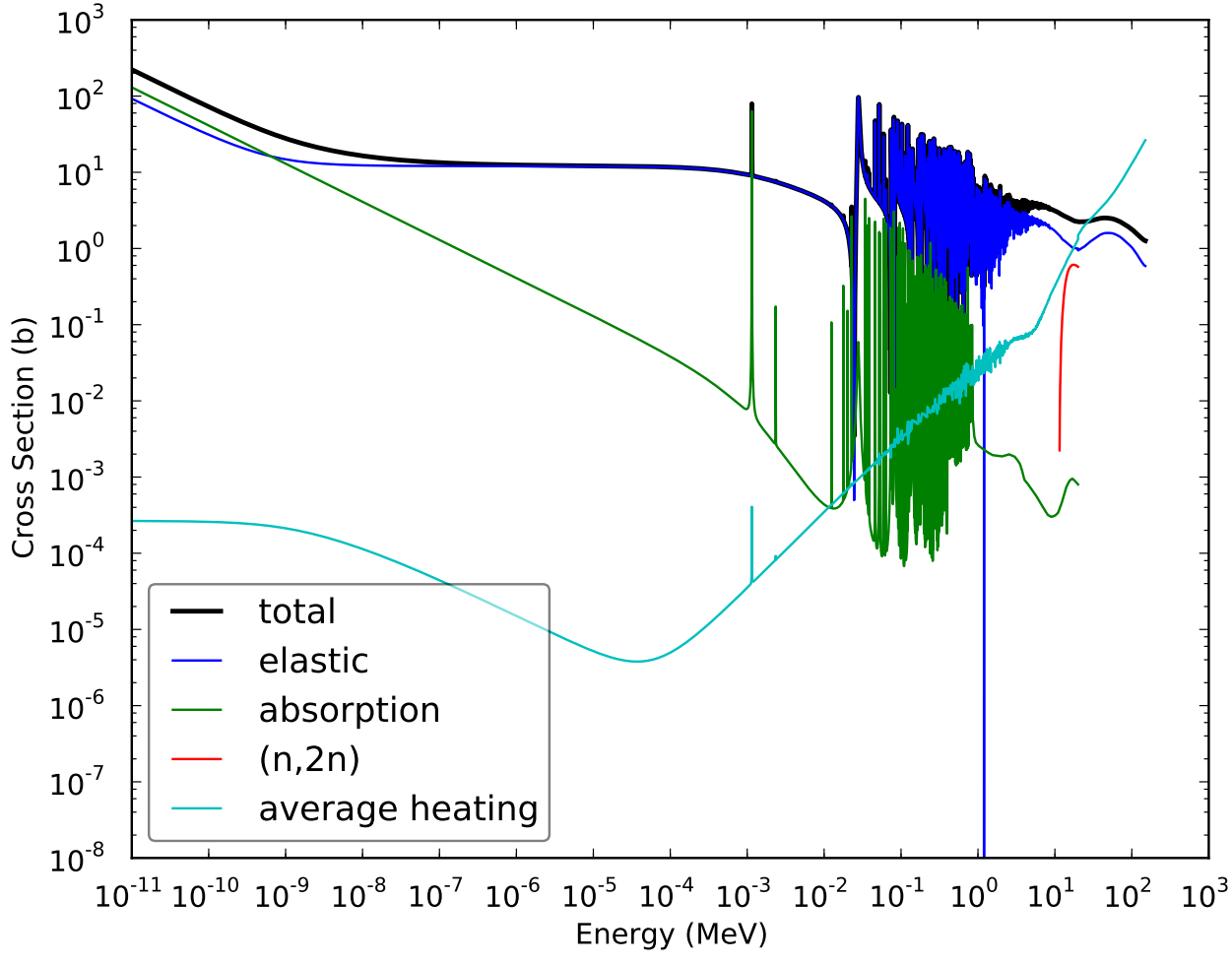
- Visual inspection
  1. σ_t, MT=1
  2. σ_a, MT=102
  3. σ_{es}, MT=2
  4. $\sigma_{(n,2n)}$, MT=16
  5. kerma*σ_t



Visual Inspection of Major Cross Sections

^{56}Fe

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



Visual Inspection of Major Cross Sections

^{123}Sn

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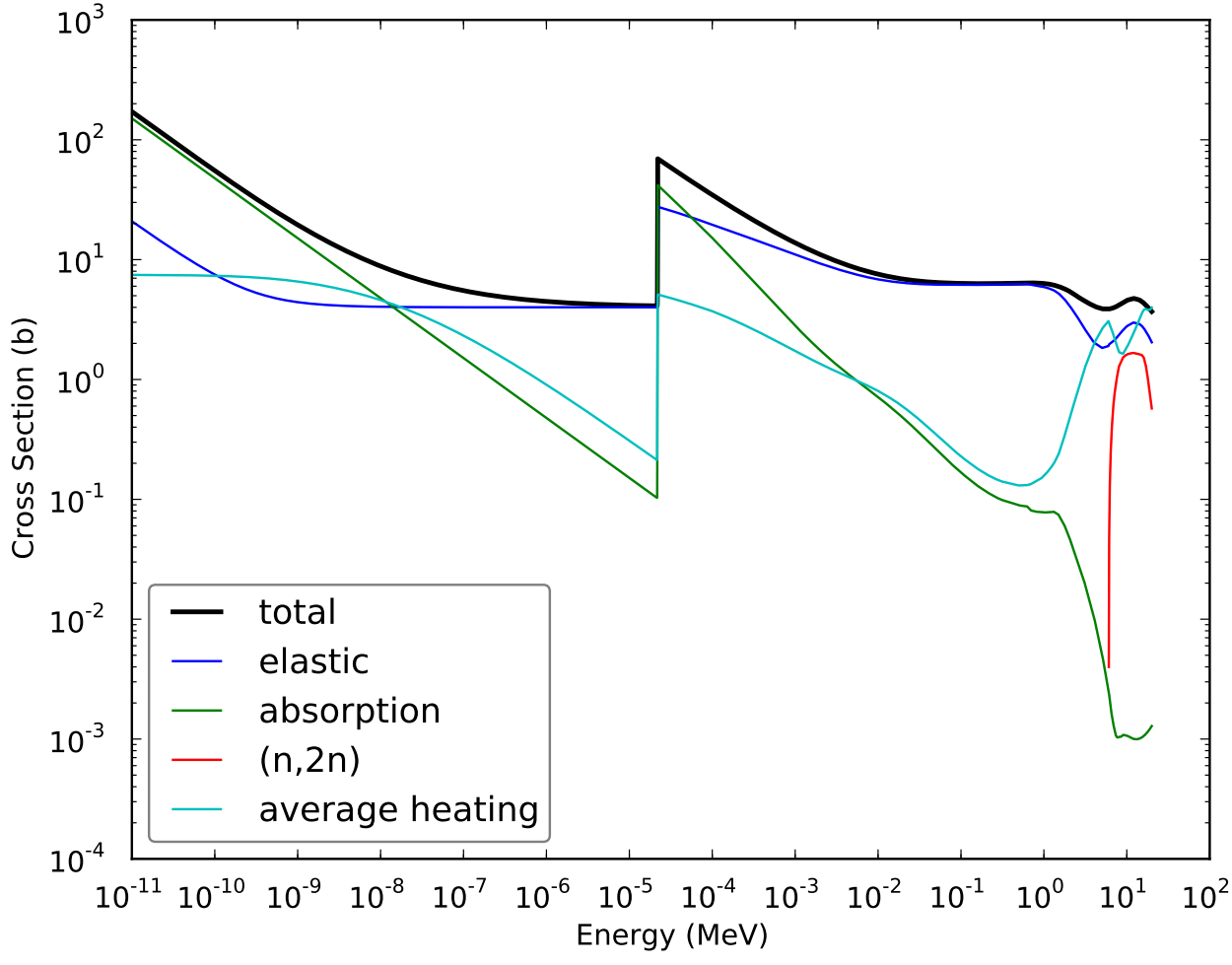
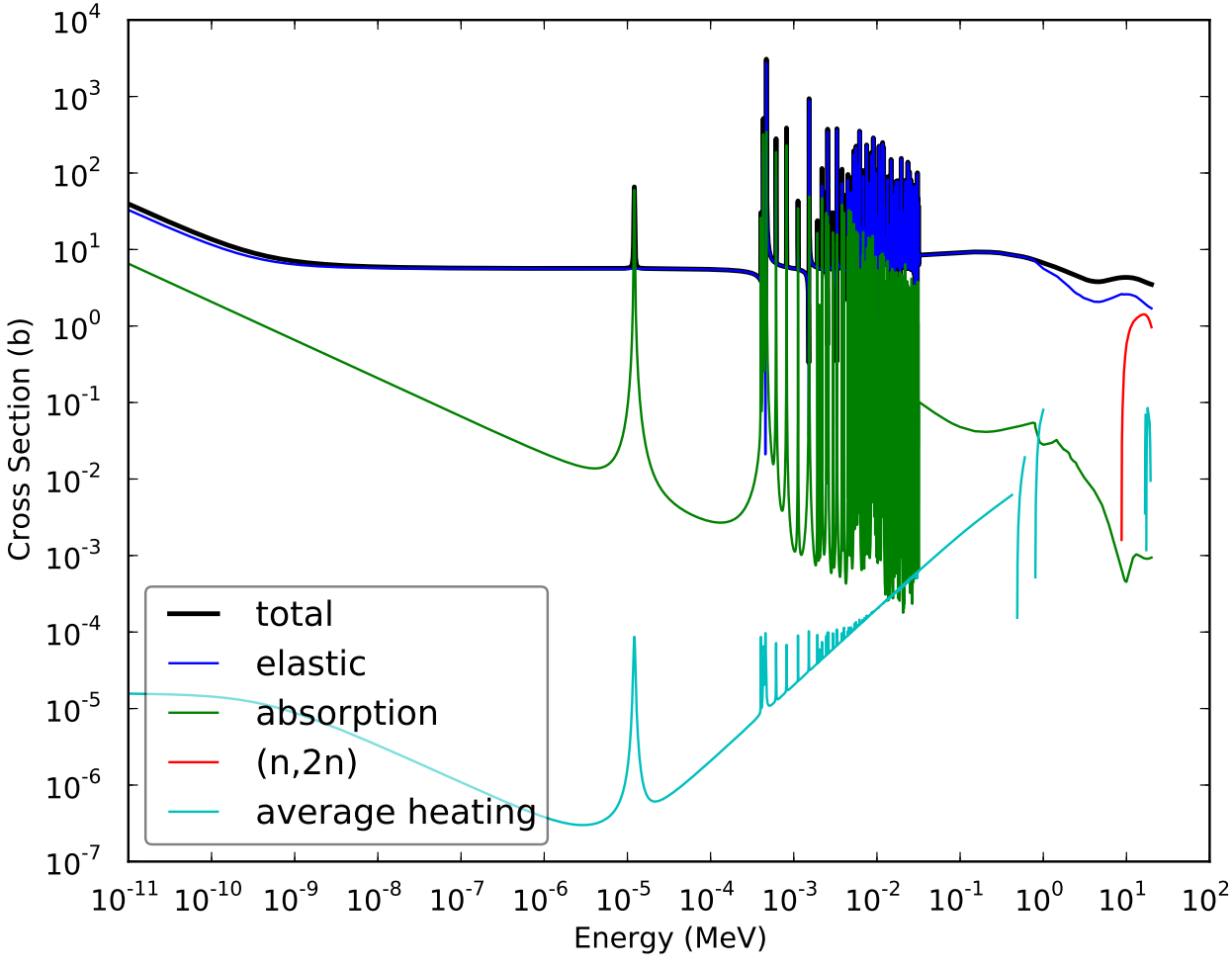
  3. σ_{es}, MT=2
  4. $\sigma_{(n,2n)}$, MT=16
  5. kerma*σ_t



Visual Inspection of Major Cross Sections

^{98}Mo

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



Changes and Additions to ENDF/B-VII.1

- ^{56}Fe and ^{61}Ni, σ_s
- ^{168}Tm
- ^{7}Be
- ^{153}Eu

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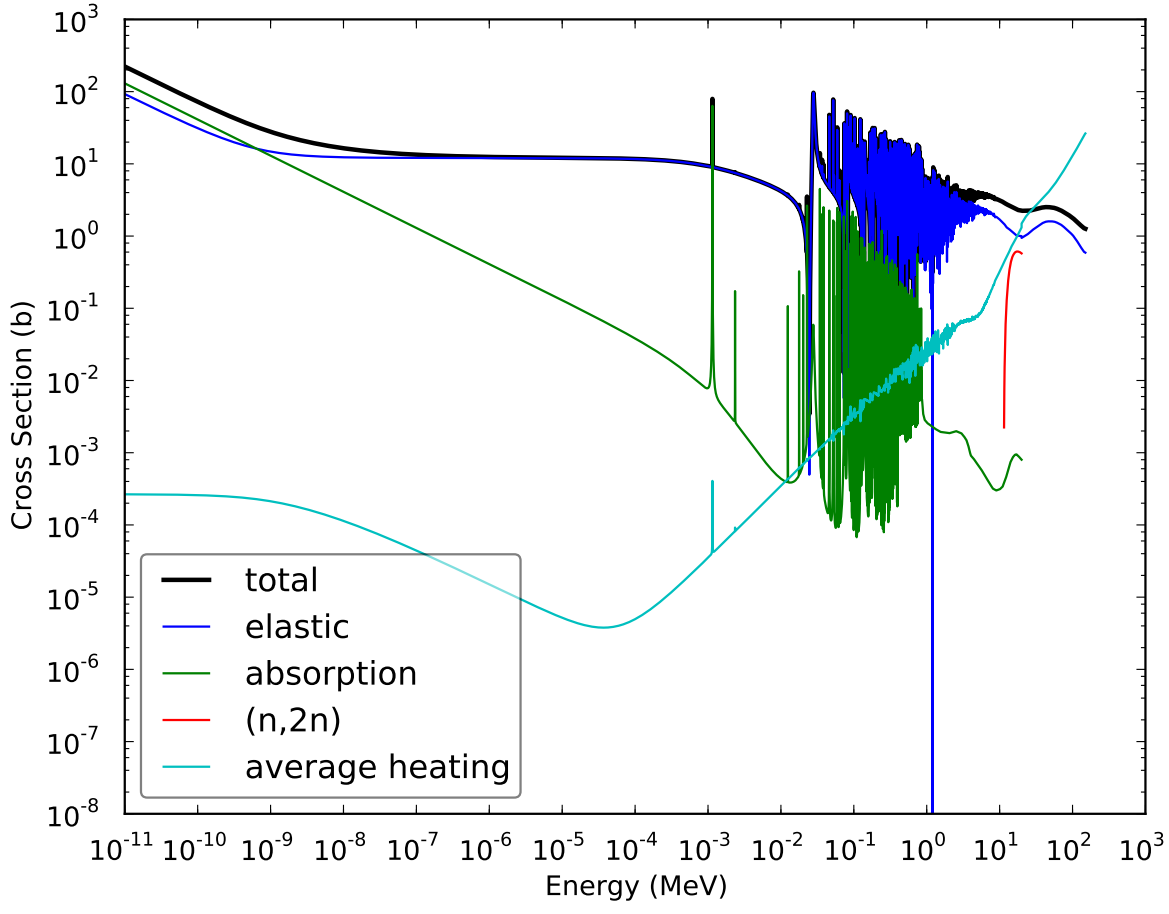


Changes and Additions to ENDF/B-VII.1

- ^{56}Fe and ^{61}Ni, σ_s
- ^{168}Tm
- ^{7}Be
- ^{153}Eu

- Error in energy-angle distribution for secondary gammas
- Affects KERMA for low incident energy neutrons
- Corrected ENDF/B file will appear in a future ENDF release

Changes and Additions to ENDF/B-VII.1

- ^{56}Fe and ^{61}Ni, σ_s
- ^{168}Tm
- ^{7}Be
- ^{153}Eu

- ENDF/B-VII.1 evaluation energies ≤ 8 MeV
- Updated to include energies ≤ 20 MeV—Should have been included in ENDF/B-VII.1
  - MENDF71x only

Changes and Additions to ENDF/B-VII.1

- ^{56}Fe and ^{61}Ni, σ_s
- ^{168}Tm
- ^{7}Be
- ^{153}Eu

- Negative PDF values were set to 0
- PDFs were renormalized

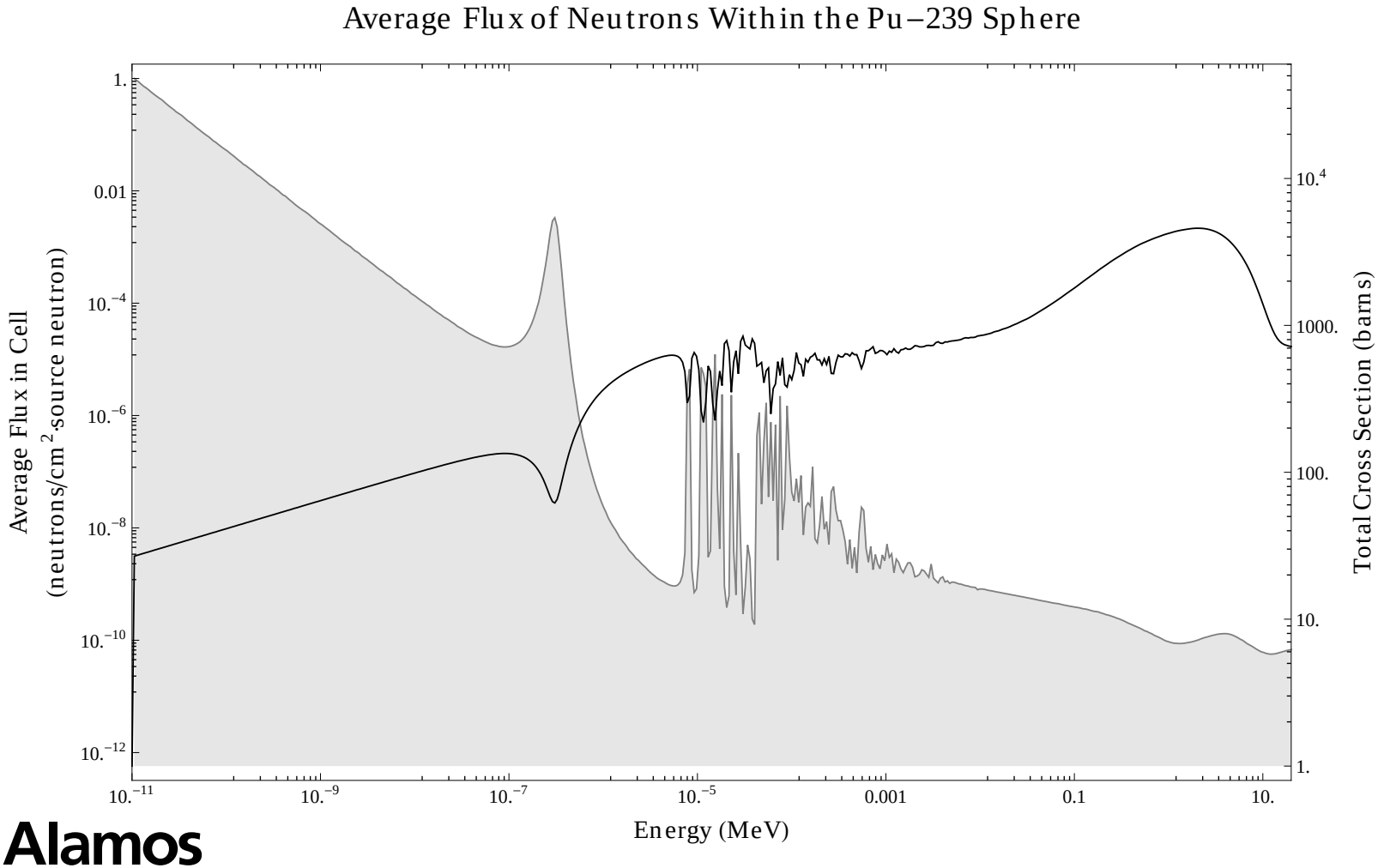
Mechanical Testing

- 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



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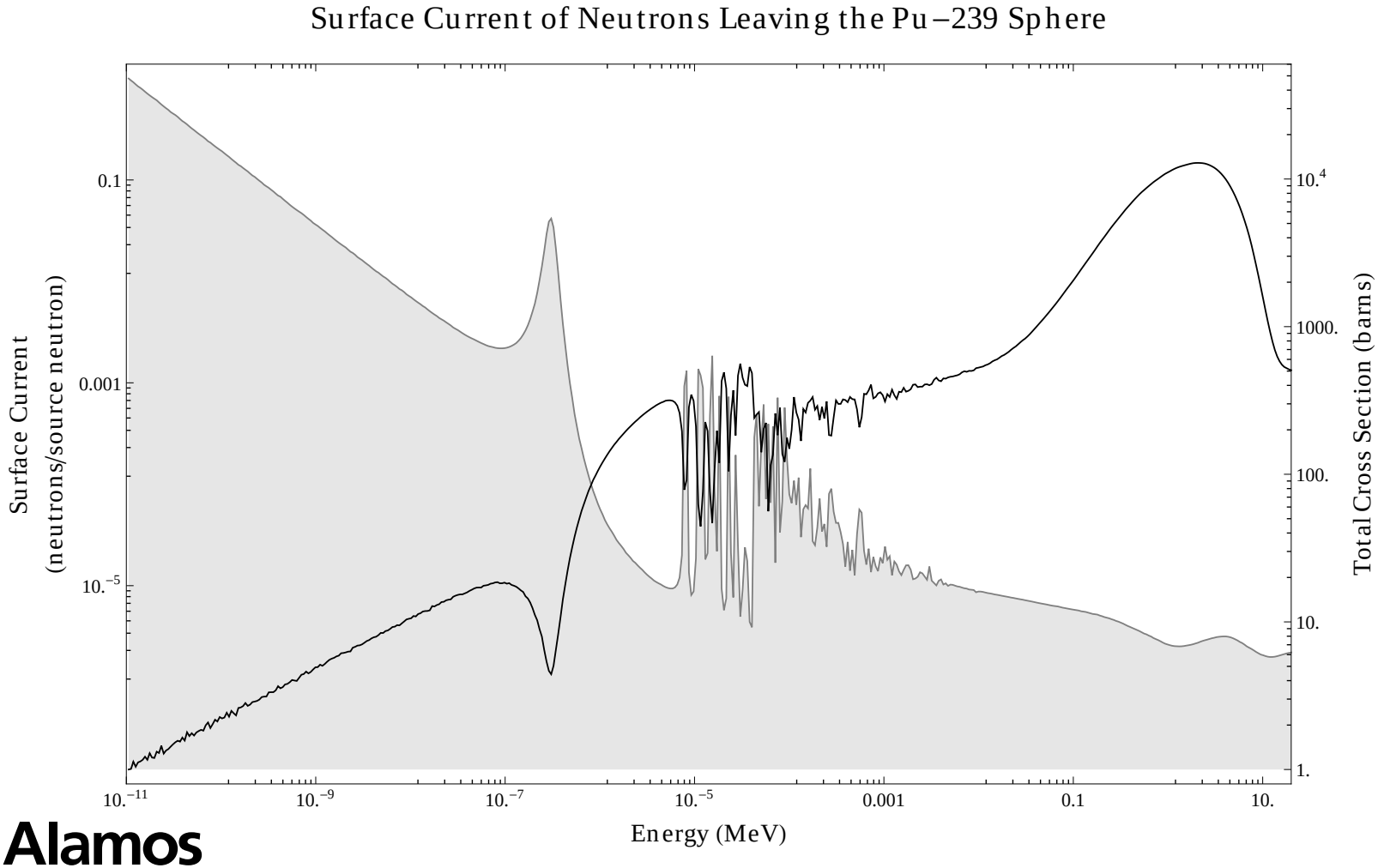
Mechanical Testing

Results



Validation using ICSBEP Benchmarks

ICSBEP

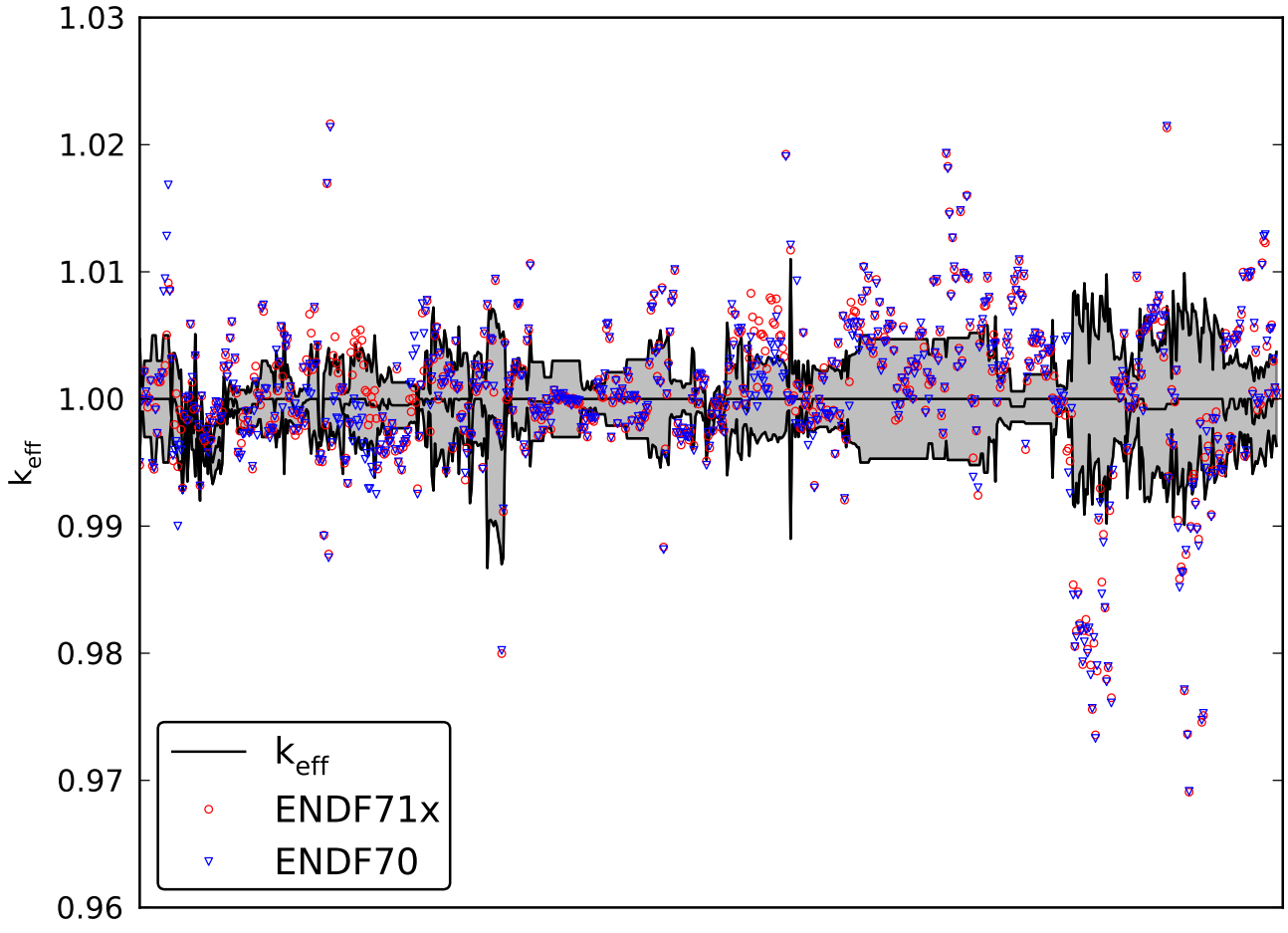
International Handbook of Evaluated Criticality Safety Benchmark Experiments

- 717 MCNP6 models (Kahler and Mosteller)
  - 18 "classes" of benchmarks
- 500 to 5000 active cycles
- 10,000 histories per cycle
- 6851 CPU hours

ICSBEP Classes of Benchmarks

Benchmark Group	#	Benchmark Group	#
HEU-COMP-INTER	1	MIX-COMP-THERM	6
HEU-MET-FAST	174	MIX-MET-FAST	34
HEU-MET-INTER	4	PU-COMP-INTER	1
HEU-MET-MIXED	5	PU-MET-FAST	43
HEU-SOL-THERM	46	PU-SOL-THERM	122
IEU-COMP-THERM	1	U233-COMP-THERM	2
IEU-MET-FAST	16	U233-MET-FAST	10
LEU-COMP-THERM	101	U233-SOL-INTER	26
LEU-SOL-THERM	22	U233-SOL-THERM	103

MCNP6 k_{eff} Results



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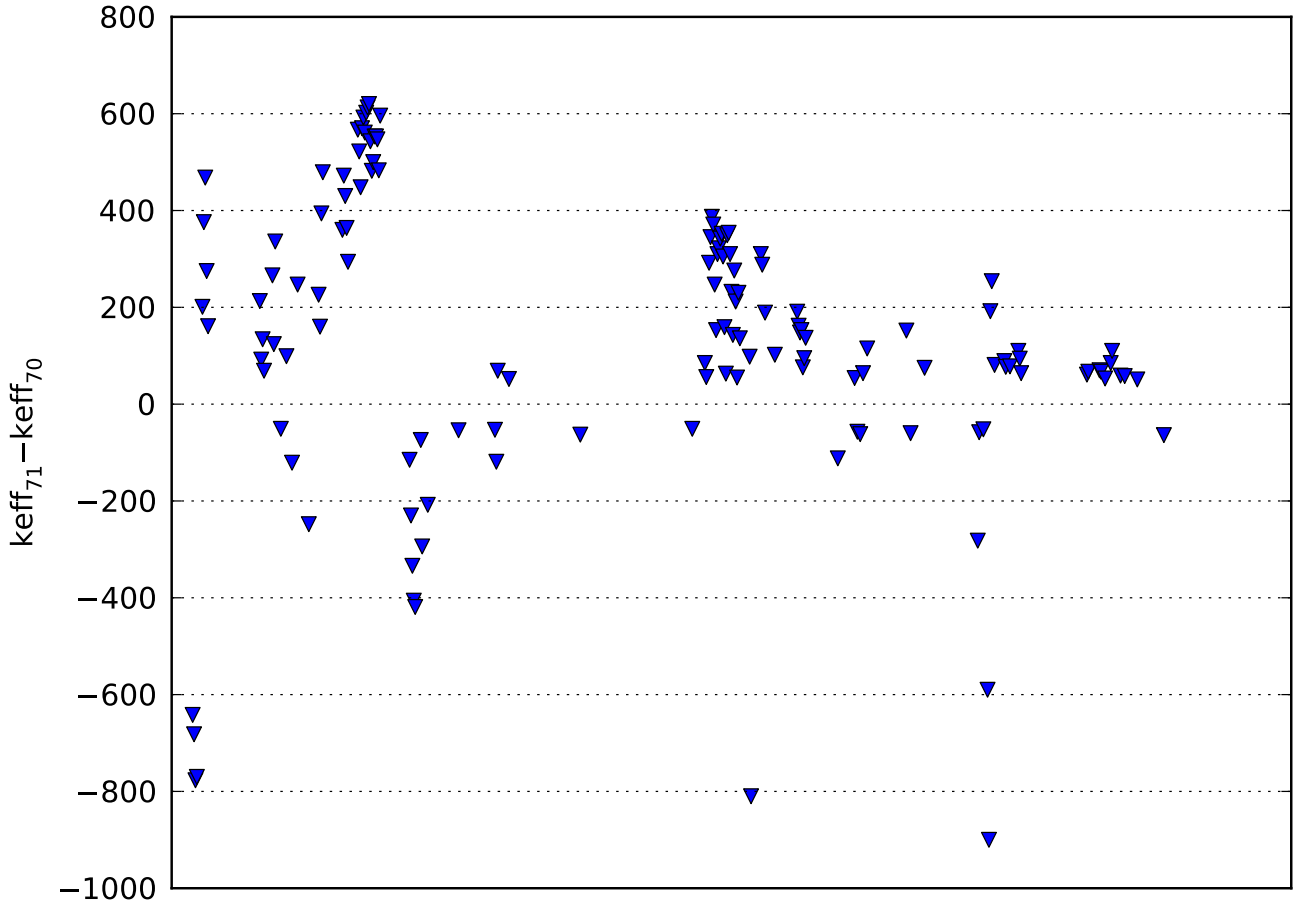

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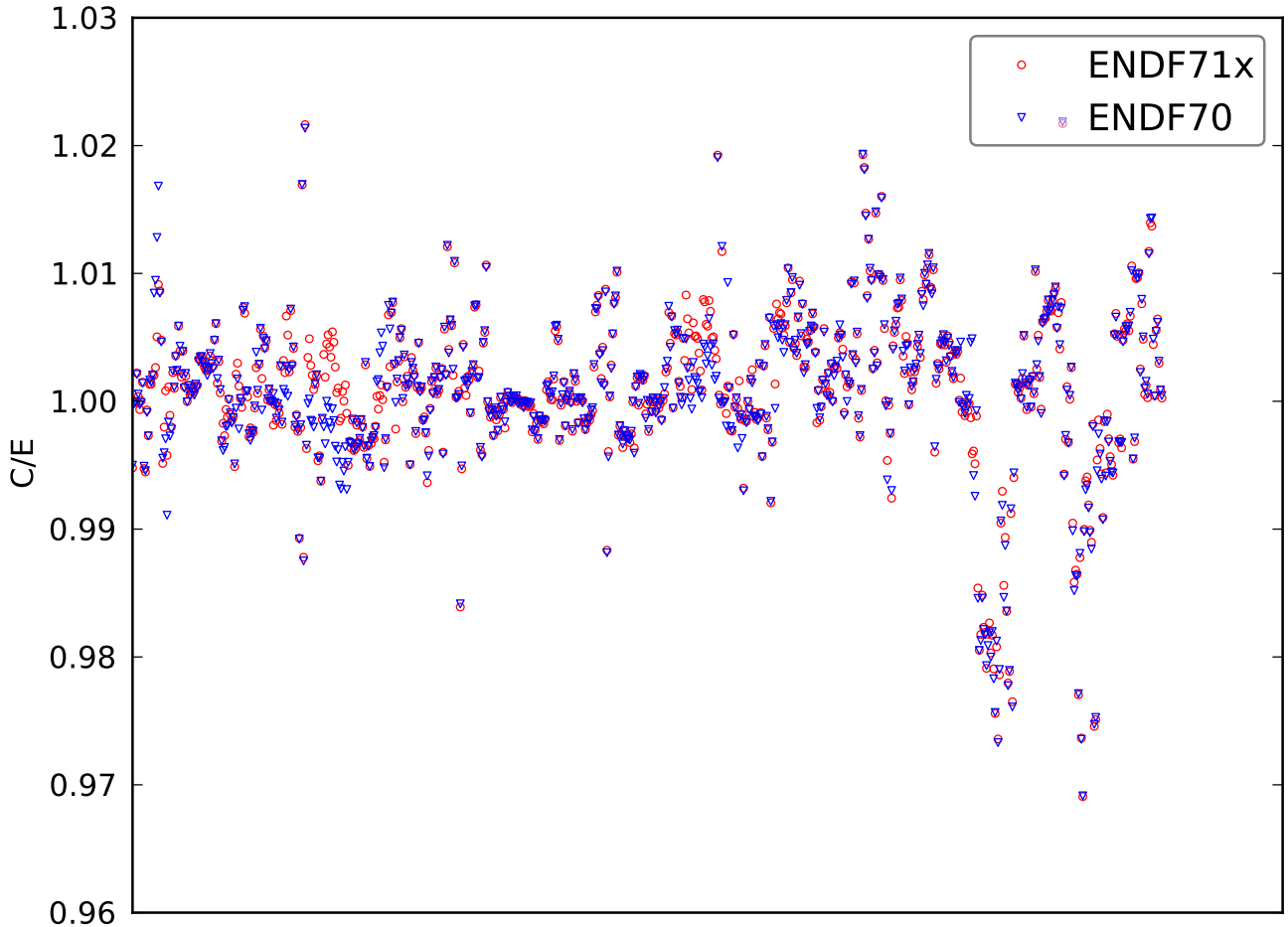
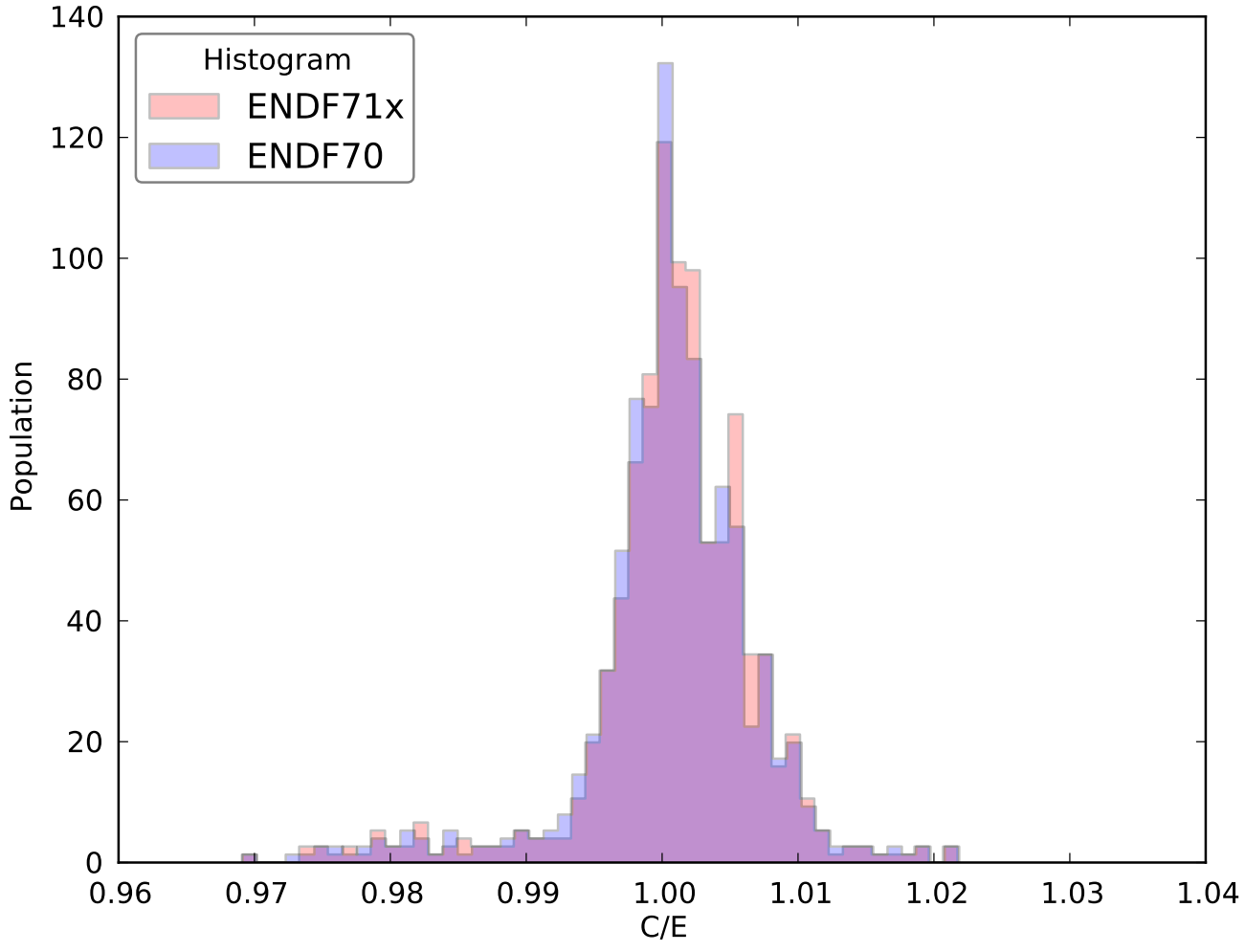


Statistical Deviations



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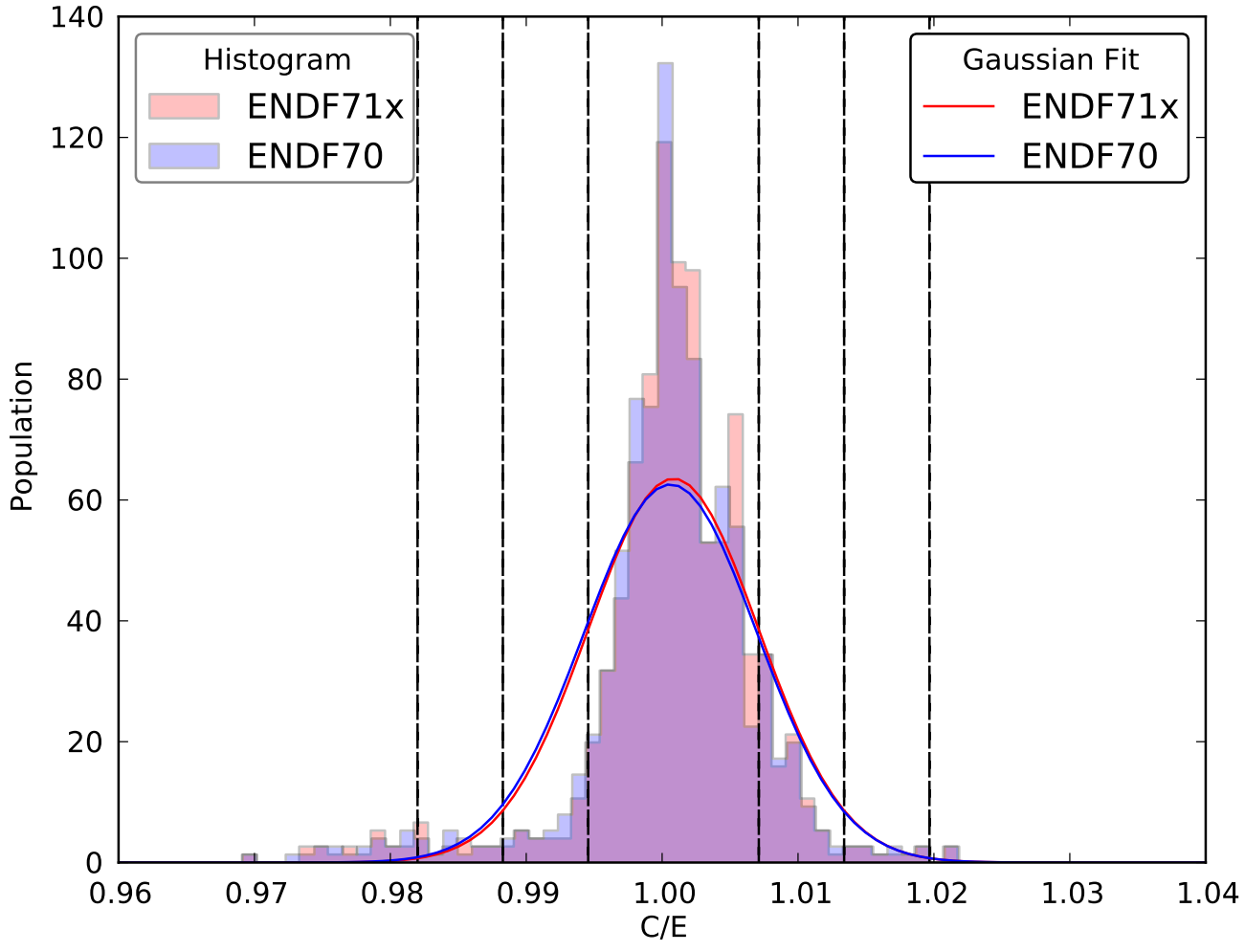
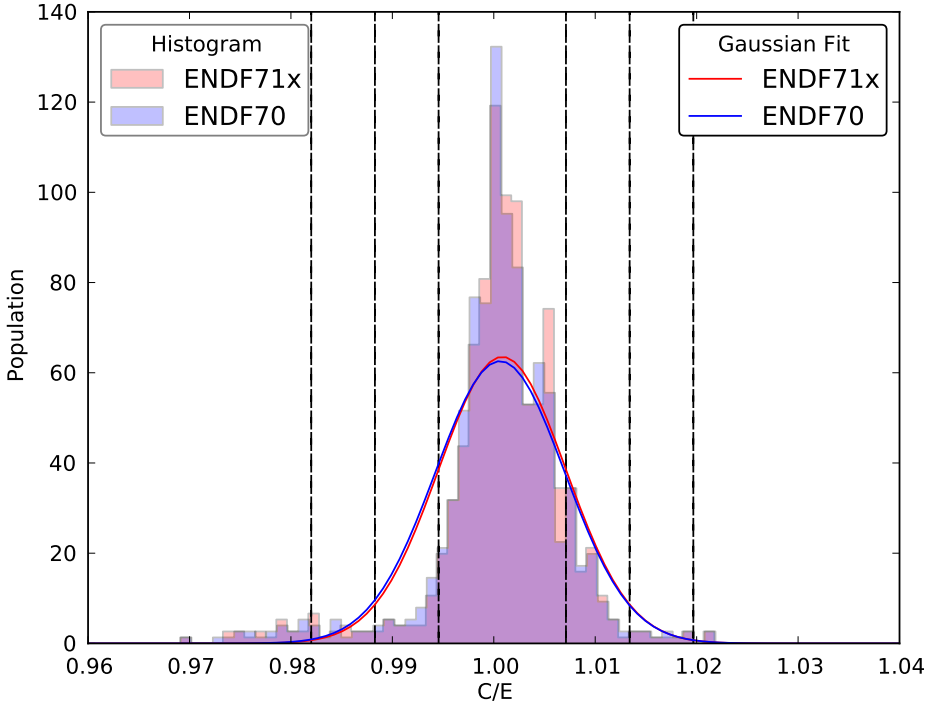


Statistical Deviations

Attempting a Gaussian Distribution



How many models fall within x standard deviations σ:

	%	Exp.	71x	70
1σ	68.3	488	335	338
2σ	95.4	682	548	550
3σ	99.7	713	642	636
4σ	99.9	714	676	674

Statistical Deviations

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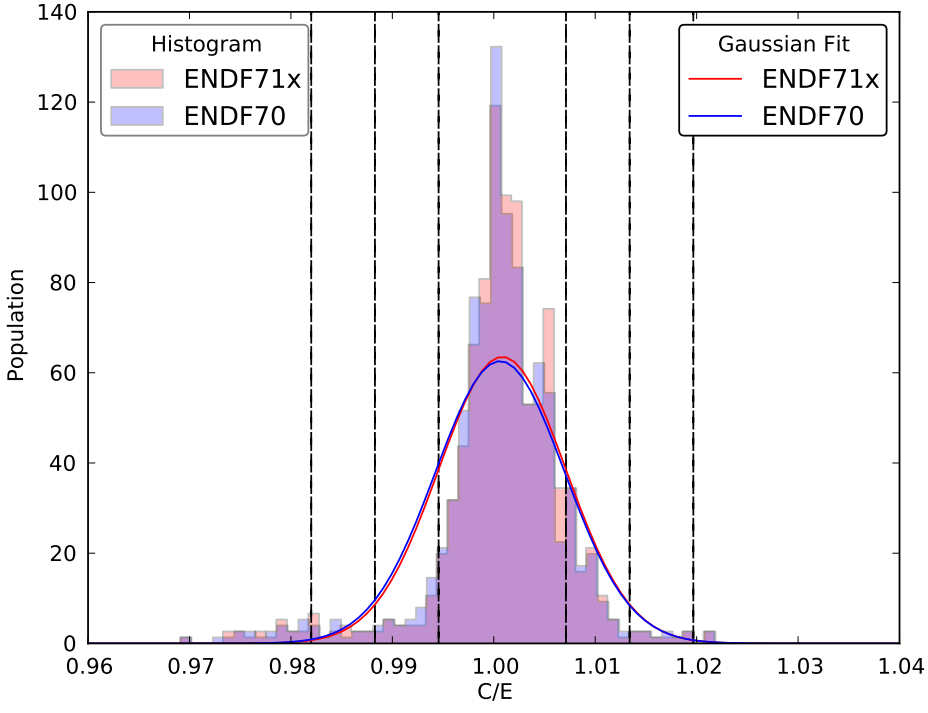

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Gaussian model is not a good fit to the data
i.e., errors not due to random fluctuations

Validation of ENDF71x

- 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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- 17,766 MCNP runs
- $> 18 \times 10^{12}$ histories
- 264,841 CPU hours

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

Data Processing Criticality Safety at LANL

ENDF/B-VII.1 and Beyond

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Data Processing Criticality Safety at LANL

ENDF/B-VII.1 and Beyond

Generalized Nuclear Data (GND):

- Modern nuclear data format
- Easily readable by humans and machines
- Avoid redundancy
- Easily extensible
- Currently underdevelopment by international organization
- Will replace ENDF-6 format and likely others, e.g., `ACE`

Data Processing Criticality Safety at LANL

ENDF/B-VII.1 and Beyond

NJOY21

NJOY for the 21st Century

- NJOY2012 tightly coupled with ENDF-6 format
- Major rewrite needed to utilize GND format

Data Processing Criticality Safety at LANL

ENDF/B-VII.1 and Beyond

NJOY21

NJOY for the 21st Century

- NJOY2012 tightly coupled with ENDF-6 format
- Major rewrite needed to utilize GND format

- Better testing—integral and unit-tests
- Better verification of nuclear data and nuclear data formats
- Faster validation of nuclear data libraries
- Extensible to future data formats

Conclusion

- Continuous-energy and multi-group-energy libraries released at LANL (ENDF71x and MENDF71x)
- ENDF71x and MENDF71x are the results of *many* hours of verification and validation
- High confidence in the quality of the nuclear data for criticality safety (and other) applications

- Significant investment in NJOY21 needed for future nuclear data processing and verification

Validation of MENDF71x with ICSBEP

Modeled k_{eff} compared to experimentally measured for 91 critical assemblies in 8 classes

HEU-MET-FAST highly enriched uranium metal, fast spectrum;

HEU-SOL-THERM highly enriched uranium in solution, thermal spectrum;

IEU-MET-FAST intermediate enriched uranium metal, fast spectrum;

MIX-MET-FAST mixed uranium and plutonium metal, fast spectrum;

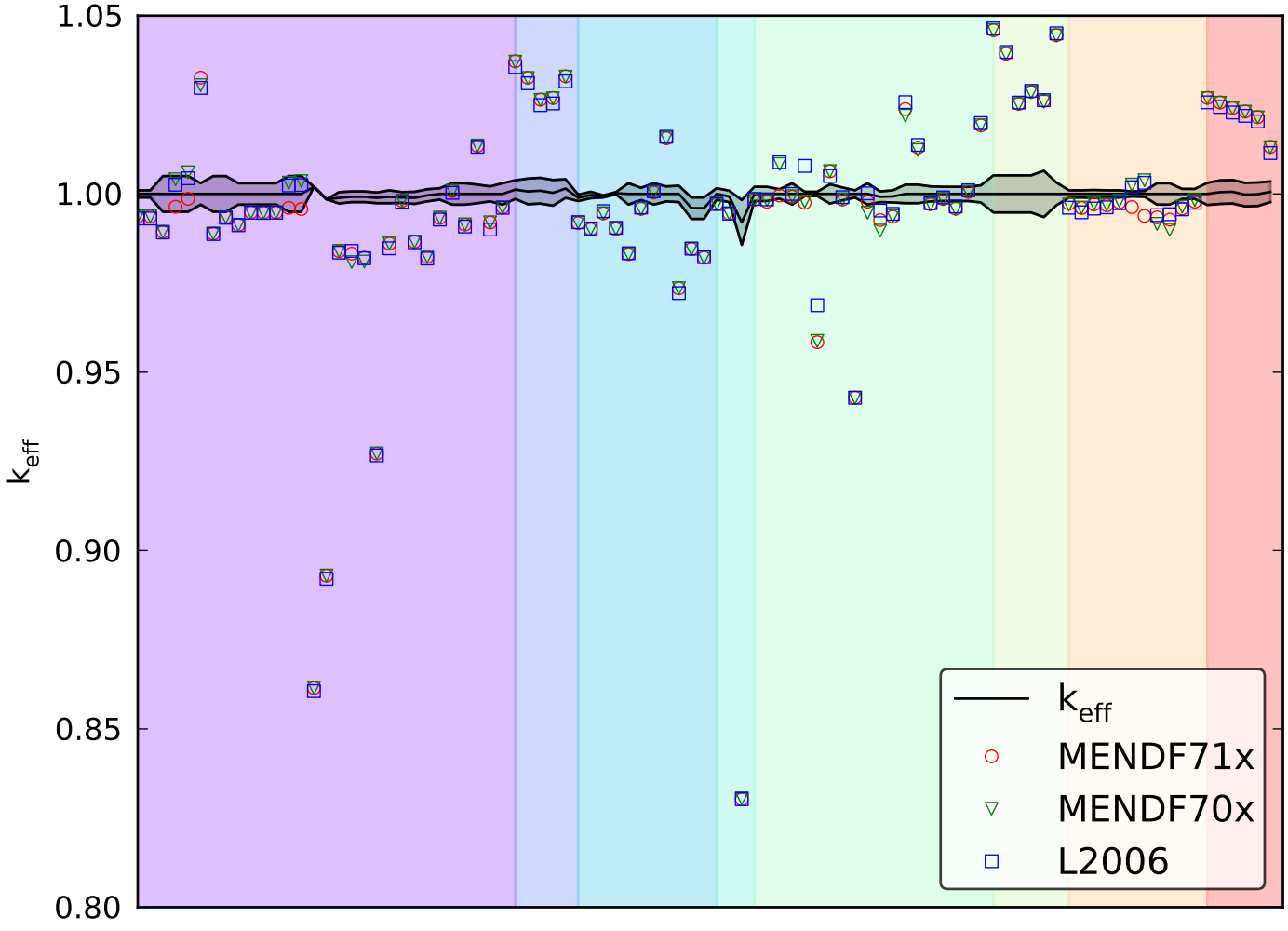
PU-MET-FAST plutonium metal, fast spectrum;

PU-SOL-THERM plutonium in solution, thermal spectrum;

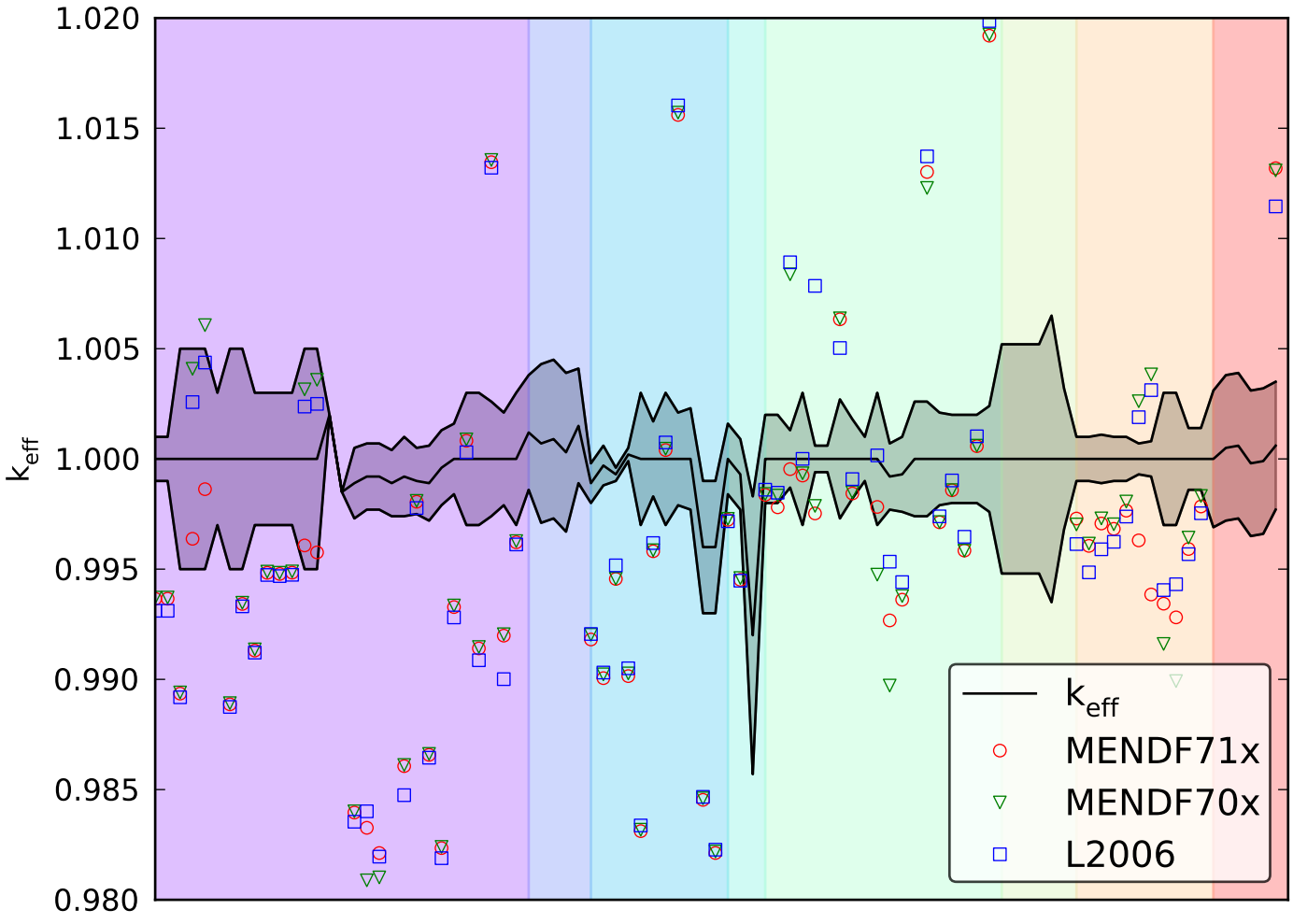
U233-MET-FAST ^{233}U metal, fast spectrum; and

U233-SOL-THERM ^{233}U in solution, thermal spectrum.

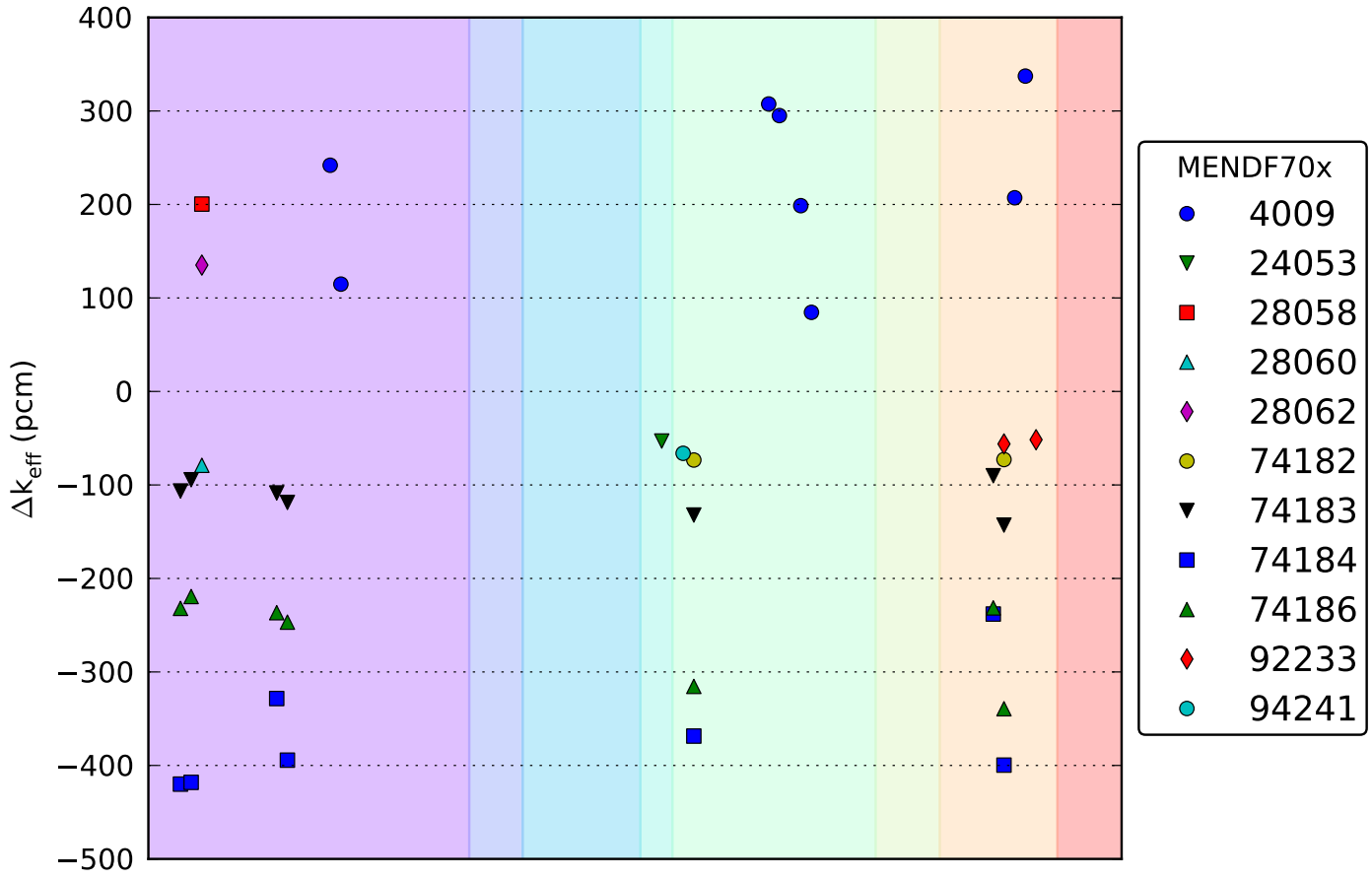
MENDF71x Validation Results



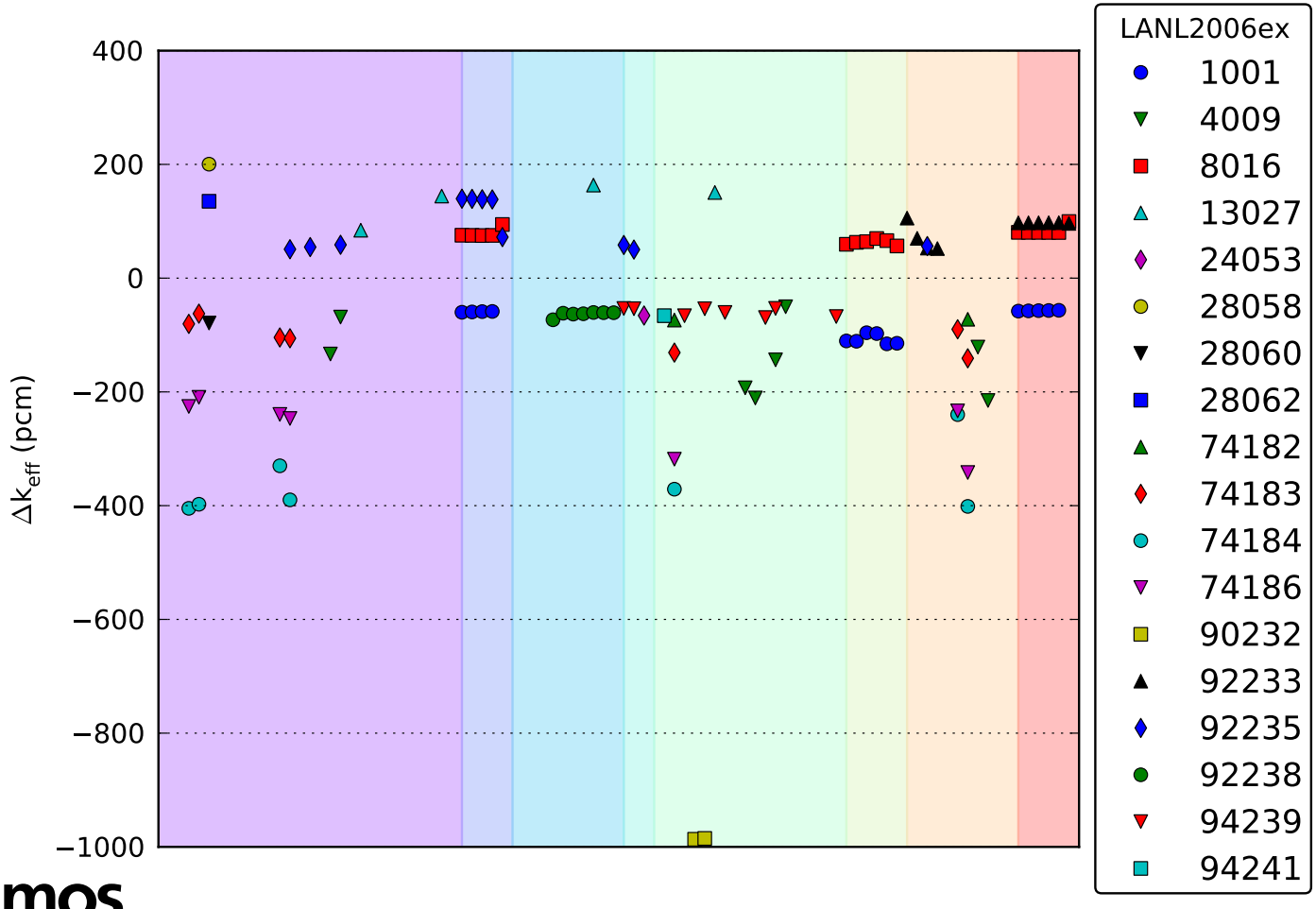
MENDF71x Validation Results



MENDF71x Validation Results—Isotopic Δk_{eff}—MENDF70x



MENDF71x Validation Results—Isotopic Δk_{eff}—LANL2006ex



MENDF71x Validation Results—Comparison to Continuous Energy Data