# Verification and Validation of MENDF71x

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## Introduction—MENDF71x

The Nuclear Data Team at Los Alamos National Laboratory has released a new, neutron transport, cross section library. The library, called MENDF71x, is based on ENDF/B-VII.1 which was released in December 2011 [1].

- 423 evaluations from ENDF/B-VII.1
- 618 groups, compatible with:
  - 250-group,
  - 133-group,
  - 70-group,
  - 30-group,
  - 21-group, and
  - 16-group.
- 293.6 K
- Infinitely dilute
- Down scatter only
- Processed with NJOY version 99.393
  - $^{35}$Cl and $^{233}$U processed with NJOY version 2012.2 [2].
- Collapsed using TD weight-function

**Most heavily verified and validated multi-group library ever released at LANL**

## Verification and Validation

### Verification

1. Do the sum of the partial cross sections equal the total cross section (`MT=1`)?
2. Do the sum of the partial fission cross sections (`MT=19,20,21,38`) equal the total fission cross section (`MT=18`)?
3. Are the chi vectors normalized to 1.0?
4. Are all the elements of the $P_0$ multi-group scattering cross sections positive?
5. Are the absolute value of the elements of the $P_l$, where $l = 1, \ldots, L$ scattering matrix less then the elements of the $P_0$ scattering matrix?
6. Are the multiplicities of the cross sections consistent with the $P_0$ Legendre scattering matrix?
7. Are the NJOY heating and KERMA cross sections consistent with those calculated by `NDI`?
   - 120 different isotopes have KERMA problems
   - none of them are *important* isotopes
8. Are the $Q-$values appropriate?

### Validation

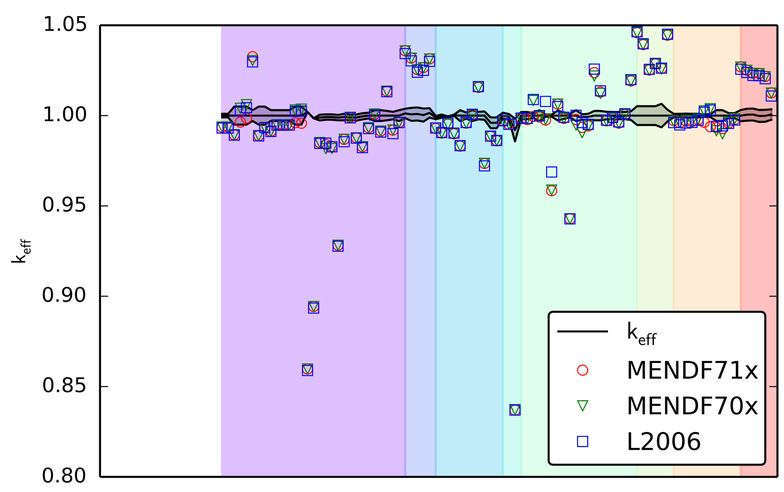
- 91 critical benchmarks from *International Handbook of Evaluated Criticality Safety Benchmark Experiments* [3].
- Benchmarks were previously studied in *A Suite of Criticality Benchmarks for Validating Nuclear Data* [4].
- Comparing modeled $k_{\text{eff}}$ values to experimentally determined $k_{\text{eff}}$ .
- Using 3 different multi-group libraries:

  **MENDF71x** based on ENDF/B-VII.1;
  **MENDF70x** based on ENDF/B-VII.0; and
  **LANL2006** based on ENDF/B-RN6.8 with evaluations added and updated in preparation for ENDF/B-VII.0.

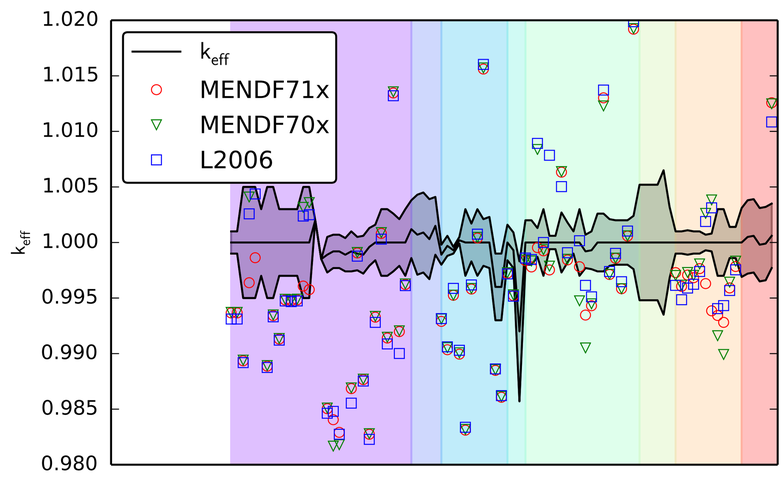
- 8 classes of benchmark models (color coded to match plots and table):

  **HEU-MET-FAST** highly enriched uranium metal with a fast spectrum;
  **HEU-SOL-THERM** highly enriched uranium in solution with a thermal spectrum;
  **IEU-MET-FAST** intermediate enriched uranium metal with a fast spectrum;
  **MIX-MET-FAST** mixed uranium and plutonium metal with a fast spectrum;
  **PU-MET-FAST** plutonium metal with fast spectrum;
  **PU-SOL-THERM** plutonium in solution with thermal spectrum;
  **U233-MET-FAST** $^{233}$U metal with fast spectrum; and
  **U233-SOL-THERM** $^{233}$U in solution with thermal spectrum.

- Shaded region in plot shows experimental $k_{\text{eff}}$ and uncertainty.




(a) Multi-group $k_{\text{eff}}$ results.




(b) Multi-group $k_{\text{eff}}$ results. Center region of Figure

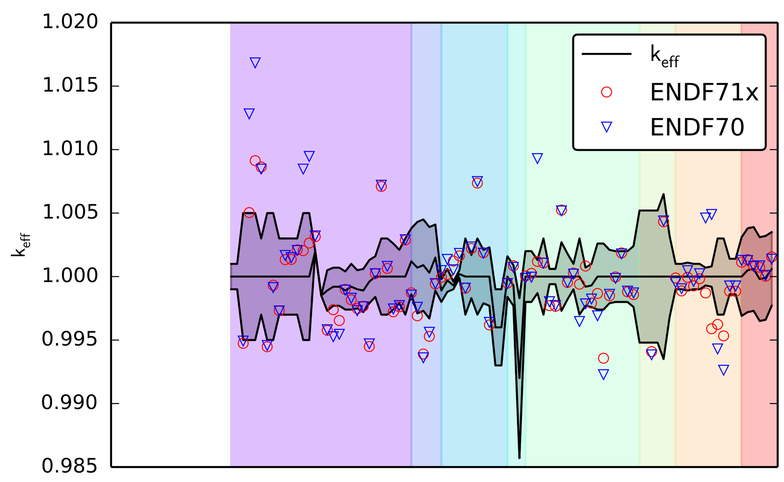
In addition to our validation with critical benchmarks, we have validated our data with other applications.

### Comparison to Monte Carlo Benchmarks

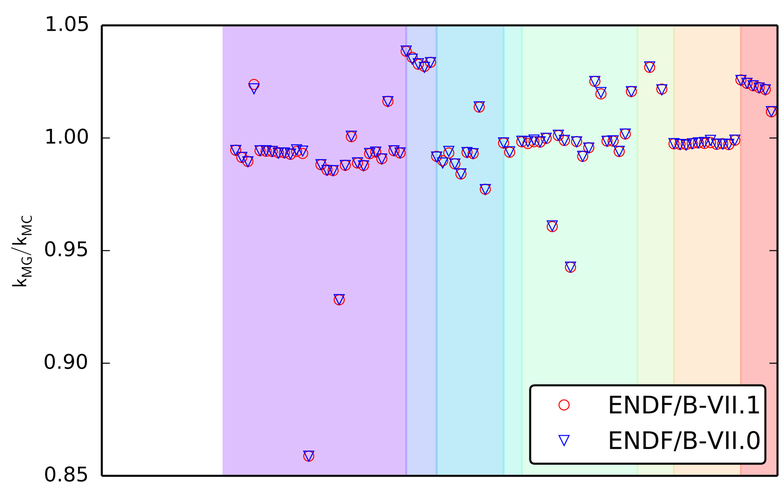
- Using 2 different continuous-energy data libraries:

  **ENDF71x** based on ENDF/B-VII.1, and
  **ENDF70** based on ENDF/B-VII.0.

- Comparing with MENDF71x and MENDF70x respectively.




(c) Monte Carlo $k_{\text{eff}}$ results.




(d) Ratio of Monte Carlo to multi-group $k_{\text{eff}}$ results.

## Comparison of $k_{\text{eff}}$ results

Red values indicate model under predicts benchmark by $\geq 10\,\%$.
Green values indicate model under predicts benchmark between $5\,\%$ to $10\,\%$
Blue values indicate model over predicts benchmark by $\geq 3\,\%$.
Shaded colors correspond to the class of benchmark and match the regions in the plots.

| # | ICSBEP Name | $k_{\text{eff}}$ Benchmark | $C/E$ Ratio MEND71x | $C/E$ Ratio MENDF70x | $C/E$ Ratio LANL2006 | $k_{MG}/k_{MC}$ MENDF71x | $k_{MG}/k_{MC}$ MENDF70x |
|---|---|---|---|---|---|---|---|
| 1 | HEU-MET-FAST-001 Case a | 1.000(1) | 0.993 66 | 0.993 71 | 0.993 11 | | |
| 2 | HEU-MET-FAST-001 Case b | 1.000(1) | 0.993 66 | 0.993 71 | 0.993 11 | | |
| 3 | HEU-MET-FAST-003 Case 1 | 1.0000(50) | 0.989 35 | 0.989 41 | 0.989 19 | 0.994 59 | 0.994 46 |
| 4 | HEU-MET-FAST-003 Case 10 | 1.0000(50) | 0.996 38 | 1.004 09 | 1.002 58 | 0.991 38 | 0.991 39 |
| 5 | HEU-MET-FAST-003 Case 11 | 1.0000(50) | 0.998 63 | 1.006 07 | 1.004 37 | 0.989 59 | 0.989 42 |
| 6 | HEU-MET-FAST-003 Case 12 | 1.0000(30) | 1.032 60 | 1.030 48 | 1.029 73 | 1.023 77 | 1.021 84 |
| 7 | HEU-MET-FAST-003 Case 2 | 1.0000(50) | 0.988 87 | 0.988 92 | 0.988 75 | 0.994 37 | 0.994 32 |
| 8 | HEU-MET-FAST-003 Case 3 | 1.0000(50) | 0.993 42 | 0.993 48 | 0.993 31 | 0.994 10 | 0.994 35 |
| 9 | HEU-MET-FAST-003 Case 4 | 1.0000(30) | 0.991 31 | 0.991 36 | 0.991 21 | 0.993 98 | 0.994 05 |
| 10 | HEU-MET-FAST-003 Case 5 | 1.0000(30) | 0.994 83 | 0.994 89 | 0.994 74 | 0.993 51 | 0.993 24 |
| 11 | HEU-MET-FAST-003 Case 6 | 1.0000(30) | 0.994 78 | 0.994 84 | 0.994 68 | 0.993 44 | 0.993 36 |
| 12 | HEU-MET-FAST-003 Case 7 | 1.0000(30) | 0.994 84 | 0.994 90 | 0.994 74 | 0.992 75 | 0.992 87 |
| 13 | HEU-MET-FAST-003 Case 8 | 1.0000(50) | 0.996 08 | 1.003 16 | 1.002 38 | 0.994 05 | 0.994 74 |
| 14 | HEU-MET-FAST-003 Case 9 | 1.0000(50) | 0.995 76 | 1.003 59 | 1.002 50 | 0.993 14 | 0.994 19 |
| 15 | HEU-MET-FAST-004 Case 1 | 1.002 00 | 0.859 72 | 0.859 75 | 0.858 88 | 0.858 75 | 0.858 72 |
| 16 | HEU-MET-FAST-004 Case 2 | 0.998 50 | 0.894 31 | 0.894 34 | 0.893 45 | | |
| 17 | HEU-MET-FAST-008 | 0.9989(16) | 0.985 04 | 0.985 10 | 0.984 63 | 0.988 14 | 0.988 15 |
| 18 | HEU-MET-FAST-009 Case 1 | 0.9992(15) | 0.984 05 | 0.981 67 | 0.984 80 | 0.985 84 | 0.985 55 |
| 19 | HEU-MET-FAST-009 Case 2 | 0.9992(15) | 0.982 91 | 0.981 80 | 0.982 74 | 0.985 53 | 0.985 50 |
| 20 | HEU-MET-FAST-011 | 0.9989(15) | 0.928 23 | 0.928 26 | 0.927 71 | 0.928 14 | 0.928 23 |
| 21 | HEU-MET-FAST-012 | 0.9992(18) | 0.986 85 | 0.986 91 | 0.985 54 | 0.987 87 | 0.987 81 |
| 22 | HEU-MET-FAST-013 | 0.9990(15) | 0.999 06 | 0.999 10 | 0.998 77 | 1.000 58 | 1.000 79 |
| 23 | HEU-MET-FAST-014 | 0.9989(17) | 0.987 66 | 0.987 70 | 0.987 53 | 0.988 89 | 0.988 97 |
| 24 | HEU-MET-FAST-015 | 0.9996(17) | 0.982 74 | 0.982 79 | 0.982 28 | 0.987 79 | 0.987 63 |
| 25 | HEU-MET-FAST-018 | 1.0000(16) | 0.993 28 | 0.993 35 | 0.992 81 | 0.993 04 | 0.993 13 |
| 26 | HEU-MET-FAST-019 | 1.0000(30) | 1.000 82 | 1.000 89 | 1.000 30 | 0.993 77 | 0.993 75 |
| 27 | HEU-MET-FAST-020 | 1.0000(30) | 0.991 40 | 0.991 47 | 0.990 87 | 0.990 77 | 0.990 68 |
| 28 | HEU-MET-FAST-021 | 1.0000(26) | 1.013 46 | 1.013 56 | 1.013 21 | 1.016 28 | 1.016 15 |
| 29 | HEU-MET-FAST-022 | 1.0000(21) | 0.991 98 | 0.992 05 | 0.990 01 | 0.994 35 | 0.994 32 |
| 30 | HEU-MET-FAST-028 | 1.0000(30) | 0.996 22 | 0.996 27 | 0.996 12 | 0.993 36 | 0.993 39 |
| 31 | HEU-SOL-THERM-013 Case 1 | 1.0012(26) | 1.035 94 | 1.035 85 | 1.034 33 | 1.038 51 | 1.038 61 |
| 32 | HEU-SOL-THERM-013 Case 2 | 1.0007(36) | 1.031 86 | 1.031 78 | 1.030 30 | 1.035 79 | 1.035 01 |
| 33 | HEU-SOL-THERM-013 Case 3 | 1.0009(36) | 1.025 52 | 1.025 44 | 1.023 98 | 1.032 74 | 1.032 97 |
| 34 | HEU-SOL-THERM-013 Case 4 | 1.0003(36) | 1.026 59 | 1.026 51 | 1.025 06 | 1.031 76 | 1.031 35 |
| 35 | HEU-SOL-THERM-032 | 1.0015(26) | 1.031 44 | 1.031 34 | 1.030 02 | 1.033 58 | 1.033 47 |
| 36 | IEU-MET-FAST-001 Case 1 | 0.9989(9) | 0.992 90 | 0.993 12 | 0.993 15 | 0.991 87 | 0.991 55 |
| 37 | IEU-MET-FAST-001 Case 2 | 0.9997(9) | 0.990 35 | 0.990 53 | 0.990 61 | 0.989 90 | 0.988 90 |
| 38 | IEU-MET-FAST-001 Case 3 | 0.9993(3) | 0.995 25 | 0.995 26 | 0.995 87 | 0.993 35 | 0.994 04 |
| 39 | IEU-MET-FAST-001 Case 4 | 1.0002(3) | 0.989 95 | 0.990 07 | 0.990 30 | 0.988 54 | 0.988 47 |
| 40 | IEU-MET-FAST-002 | 1.000(3) | 0.983 11 | 0.983 18 | 0.983 37 | 0.984 01 | 0.984 08 |
| 41 | IEU-MET-FAST-003 | 1.0000(17) | 0.995 81 | 0.995 86 | 0.996 18 | 0.993 62 | 0.993 55 |
| 42 | IEU-MET-FAST-004 | 1.0000(30) | 1.000 40 | 1.000 46 | 1.000 75 | 0.993 09 | 0.993 03 |
| 43 | IEU-MET-FAST-005 | 1.0000(21) | 1.015 61 | 1.015 71 | 1.016 03 | 1.013 70 | 1.013 85 |
| 44 | IEU-MET-FAST-006 | 1.0000(23) | 0.973 52 | 0.973 57 | 0.972 18 | 0.977 25 | 0.977 10 |
| 45 | IEU-MET-FAST-007 | 0.996(3) | 0.986 07 | 0.986 14 | 0.986 22 | | |
| 46 | IEU-MET-FAST-007 | 0.996(3) | 0.988 49 | 0.988 56 | 0.988 62 | | |
| 47 | MIX-MET-FAST-001 | 1.0000(16) | 0.997 24 | 0.997 28 | 0.997 17 | 0.997 75 | 0.997 83 |
| 48 | MIX-MET-FAST-003 | 0.9993(16) | 0.995 21 | 0.995 29 | 0.995 17 | 0.993 67 | 0.993 88 |
| 49 | MIX-MET-FAST-008 Case 1 | 0.9920(63) | 0.836 95 | 0.837 24 | 0.836 98 | | |
| 50 | PU-MET-FAST-001 | 1.000(2) | 0.998 37 | 0.998 41 | 0.998 60 | 0.998 32 | 0.998 55 |
| 51 | PU-MET-FAST-002 | 1.000(2) | 0.997 80 | 0.998 34 | 0.998 47 | 0.997 56 | 0.998 39 |
| 52 | PU-MET-FAST-005 | 1.0000(13) | 0.999 54 | 1.008 37 | 1.008 92 | 0.998 35 | 0.999 09 |
| 53 | PU-MET-FAST-006 | 1.0000(30) | 0.999 25 | 0.999 35 | 1.000 00 | 0.998 18 | 0.998 30 |
| 54 | PU-MET-FAST-008 Case 1 | 1.0000(6) | 0.997 53 | 0.997 87 | 1.007 85 | 0.999 82 | 0.999 85 |
| 55 | PU-MET-FAST-008 Case 2 | 1.0000(6) | 0.958 41 | 0.958 78 | 0.968 77 | 0.960 66 | 0.960 97 |
| 56 | PU-MET-FAST-009 | 1.0000(27) | 1.006 33 | 1.006 38 | 1.005 03 | 1.001 09 | 1.001 20 |
| 57 | PU-MET-FAST-010 | 1.0000(18) | 0.998 43 | 0.998 49 | 0.999 08 | 0.998 89 | 0.998 95 |
| 58 | PU-MET-FAST-011 | 1.0000(10) | 0.942 86 | 0.942 84 | 0.942 84 | 0.942 60 | 0.942 66 |
| 59 | PU-MET-FAST-018 | 1.0000(30) | 0.997 82 | 0.994 75 | 1.000 16 | 0.998 42 | 0.998 28 |
| 60 | PU-MET-FAST-019 | 0.9992(15) | 0.993 47 | 0.990 51 | 0.996 14 | 0.991 85 | 0.991 85 |
| 61 | PU-MET-FAST-020 | 0.9993(17) | 0.994 31 | 0.994 48 | 0.995 11 | 0.995 69 | 0.995 54 |
| 62 | PU-MET-FAST-021 Case 1 | 1.0000(26) | 1.023 79 | 1.021 92 | 1.025 73 | 1.025 15 | 1.025 09 |
| 63 | PU-MET-FAST-021 Case 2 | 1.0000(26) | 1.013 02 | 1.012 29 | 1.013 72 | 1.019 57 | 1.020 18 |
| 64 | PU-MET-FAST-022 | 1.0000(21) | 0.997 12 | 0.997 14 | 0.997 39 | 0.998 63 | 0.998 54 |
| 65 | PU-MET-FAST-023 | 1.0000(20) | 0.998 58 | 0.998 59 | 0.999 02 | 0.998 61 | 0.998 74 |
| 66 | PU-MET-FAST-024 | 1.0000(20) | 0.995 84 | 0.995 84 | 0.996 47 | 0.993 99 | 0.994 07 |
| 67 | PU-MET-FAST-025 | 1.0000(20) | 1.000 58 | 1.000 60 | 1.001 03 | 1.001 78 | 1.001 75 |
| 68 | PU-MET-FAST-026 | 1.0000(24) | 1.019 20 | 1.019 25 | 1.019 87 | 1.020 65 | 1.020 57 |
| 69 | PU-SOL-THERM-011 Case 16-1 | 1.0000(52) | 1.045 90 | 1.045 89 | 1.046 41 | | |
| 70 | PU-SOL-THERM-011 Case 16-5 | 1.0000(52) | 1.039 32 | 1.039 33 | 1.039 80 | | |
| 71 | PU-SOL-THERM-011 Case 18-1 | 1.0000(52) | 1.025 26 | 1.025 20 | 1.025 61 | 1.031 36 | 1.031 57 |
| 72 | PU-SOL-THERM-011 Case 18-6 | 1.0000(52) | 1.028 59 | 1.028 54 | 1.028 89 | | |
| 73 | PU-SOL-THERM-021 Case 3 | 1.0000(65) | 1.026 12 | 1.025 86 | 1.026 29 | 1.021 71 | 1.021 39 |
| 74 | PU-SOL-THERM-021 Case 7 | 1.0000(32) | 1.044 50 | 1.044 45 | 1.045 03 | | |
| 75 | U233-MET-FAST-001 | 1.000(1) | 0.997 29 | 0.997 03 | 0.996 14 | 0.997 41 | 0.997 50 |
| 76 | U233-MET-FAST-002 Case 1 | 1.0000(10) | 0.996 05 | 0.996 16 | 0.994 85 | 0.997 18 | 0.997 12 |
| 77 | U233-MET-FAST-002 Case 2 | 1.0000(11) | 0.997 07 | 0.997 30 | 0.995 90 | 0.997 13 | 0.996 84 |
| 78 | U233-MET-FAST-003 Case 1 | 1.0000(10) | 0.996 83 | 0.997 04 | 0.996 24 | 0.997 56 | 0.997 42 |
| 79 | U233-MET-FAST-003 Case 2 | 1.0000(10) | 0.997 65 | 0.998 07 | 0.997 39 | 0.997 82 | 0.997 85 |
| 80 | U233-MET-FAST-004 Case 1 | 1.0000(7) | 0.996 30 | 1.002 62 | 1.001 89 | 0.997 59 | 0.998 02 |
| 81 | U233-MET-FAST-004 Case 2 | 1.0000(8) | 0.993 85 | 1.003 83 | 1.003 12 | 0.997 95 | 0.998 95 |
| 82 | U233-MET-FAST-005 Case 1 | 1.0000(30) | 0.993 43 | 0.991 61 | 0.994 05 | 0.997 19 | 0.997 30 |
| 83 | U233-MET-FAST-005 Case 2 | 1.0000(30) | 0.992 81 | 0.989 92 | 0.994 32 | 0.997 47 | 0.997 28 |
| 84 | U233-MET-FAST-006 | 1.0000(14) | 0.997 84 | 0.998 32 | 0.997 54 | 0.997 07 | 0.997 17 |
| 85 | U233-MET-FAST-006 | 1.0000(14) | 0.995 91 | 0.996 43 | 0.995 68 | 0.999 00 | 0.999 06 |
| 86 | U233-SOL-THERM-001 Case 1 | 1.0000(31) | 1.026 94 | 1.026 86 | 1.025 68 | 1.025 78 | 1.025 56 |
| 87 | U233-SOL-THERM-001 Case 2 | 1.0005(33) | 1.025 13 | 1.025 05 | 1.023 88 | 1.024 27 | 1.024 27 |
| 88 | U233-SOL-THERM-001 Case 3 | 1.0006(33) | 1.023 46 | 1.023 38 | 1.022 22 | 1.023 20 | 1.023 18 |
| 89 | U233-SOL-THERM-001 Case 4 | 0.9998(33) | 1.023 33 | 1.023 25 | 1.022 09 | 1.022 38 | 1.022 18 |
| 90 | U233-SOL-THERM-001 Case 5 | 0.9999(33) | 1.021 65 | 1.021 57 | 1.020 42 | 1.021 52 | 1.021 38 |
| 91 | U233-SOL-THERM-008 | 1.0006(29) | 1.012 58 | 1.012 48 | 1.010 85 | 1.011 62 | 1.011 70 |

## Conclusion

- Most heavily verified and validated multi-group neutron transport library ever released at LANL.
- Modest improvement over MENDF70x and LANL2006 libraries.
- ENDF/B-VII.1 has many problems with KERMA data, but not in important isotopes.
- Most modeled $k_{\text{eff}}$ values fall within a few % of the experimental benchmark $k_{\text{eff}}$ and Monte Carlo calculation.
- Benchmarks with thermal spectrum are difficult to match with multi-group models because of these limitations of MENDF71x:
  - TD weight-function not optimal for thermal spectrum,
  - lack of $S(\alpha, \beta)$ effects,
  - lack of upscatter,
  - lack of resonance self-shielding data.
- Foundation for future multi-group, multi-temperature library.

## Acknowledgements

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## References

M.B. Chadwick et al. "ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data". In: *Nuclear Data Sheets* 112.12 (2011), pp. 2887–2996.

A. C. Kahler et al. *The NJOY Nuclear Data Processing System, Version 2012*. Los Alamos National Laboratory, Theoretical Division. Dec. 2012.

J. Blair Briggs. *International Handbook of Evaluated Criticality Safety Benchmark Experiments*. September 2011. Nuclear Energy Agency (AEN/NEA), 2011.

Stephanie C. Frankle. *A Suite of Criticality Benchmarks for Validating Nuclear Data*. Tech. rep. LA-13594. Los Alamos National Laboratory, Apr. 1999.

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