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Title: An Expanded Criticality Validation Suite for MCNP

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An Expanded Criticality Validation Suite for MCNP

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"International Conference on Nuclear Criticality"
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An expanded criticality validation suite has been created for the MCNP Monte Carlo code. The suite includes 119 benchmarks taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments*. The 119 benchmarks are divided into five categories of fuel – ^{233}U, highly enriched uranium (HEU), intermediate enriched uranium (IEU), low enriched uranium (LEU), and plutonium. The ^{233}U, HEU, IEU, and plutonium benchmarks are subdivided farther according to spectrum – fast, intermediate, or thermal. The LEU category contains only thermal cases, since LEU can reach criticality only with a thermal spectrum. Succinct descriptions are provided for each benchmark, along with computed values for k_{eff} for selected cases using nuclear data libraries based on ENDF/B-VII.0 and ENDF/B-VII.1β3.

An Expanded Criticality Validation Suite for MCNP

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Overview of Presentation

Introductory comments

Computer code verification and validation

MCNP validation suites

Expanded Criticality Validation Suite

Succinct description of the the benchmarks in the Expanded Criticality Validation Suite

Selected results from ENDF/B-VII.0 and ENDF/B-VII.1β3

Summary

Introductory Comments

If you don't validate your computer tools,
your results are worthless

If you don't document your V&V work,
your results are worthless

If you don't document your work,
it is worthless

Verification and validation are not glamorous or fun, but they are absolutely necessary

You still must validate even well-known codes (e.g., MCNP, SCALE) for your particular applications

Computer Code Verification and Validation (1)

Criticality safety practitioners are required to validate the computational tools used in their work, and so are code developers

Criticality Safety Practitioners

Identify a set of experimental bench-marks similar to the problem of interest

Analyze the benchmarks with the code

Assess the accuracy of computed results versus benchmark values

Focus:
Determine whether a general-purpose tool performs adequately for a specific problem of interest

Code Developers

Identify a set of experimental benchmarks that span all types of problems that users may run

Analyze the benchmarks with the code

Assess the accuracy of computed results versus benchmark values

Focus:
Determine whether the code performs properly for a wide range of problems

Computer Code Verification and Validation (2)

<u>Verification</u>

Confirm that the code faithfully solves the equations and physical models it was designed to solve

Test with a series of calculations and comparisons with closed-form analytic solutions and with reference results from previously verified codes

<u>Validation</u>

Confirm that the code faithfully reproduces reality for a particular range of applicability

Confirm that the code bounds end-user applications

Compare calculational results with relevant benchmark values

Possibly perform scoping studies to ensure that parameter changes produce expected changes in results

Computer Code Verification and Validation (3)

While code developers can thoroughly verify their codes, validation is problematic because of the very wide range of applications and multiple code options

Validation performed by code developers necessarily must be general, involving suites of problems chosen to broadly represent and span the range of possible applications

MCNP Verification and Validation Suites

More than a dozen verification and validation suites have been developed for the MCNP Monte Carlo code, including

- Regression / Installation
- Criticality
- Radiation Shielding / Dose
- Electrons
- Photons
- Variance Reduction
- Rossi α (described in a paper on Wednesday morning)

The suites provide a general indication of the overall performance of MCNP with any of a number of nuclear data libraries, and they can alert the user to unexpected or unintended consequences resulting from changes to nuclear data or to the code itself

This presentation focuses on the validation of MCNP for criticality safety and reactor applications

MCNP Criticality Validation Suites

For several years, the nuclear data and Monte Carlo teams at LANL each have had its own MCNP validation suite

Nuclear Data Team Validation Suite

Used primarily for nuclear data testing

Contains 93 benchmarks, but all are fast metal or thermal solution systems

Specifications for most of the benchmarks are taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* or from the CSEWG Benchmark Book

Includes several sets of related benchmarks so that effects of parameter variations (reflector thickness, solution content, etc.) may be evaluated

Monte Carlo Team Validation Suite

Used primarily to test changes to MCNP and its nuclear data libraries

Contains 31 benchmarks, including fast, intermediate, and thermal spectra as well as a variety of fuel materials and geometries

All input specifications are taken from the *Handbook*

Does not include sets of related benchmarks for parameter studies

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Expanded Criticality Validation Suite (1)

Includes many of the benchmarks in the Nuclear Data and Monte Carlo team suites

Eliminates overlaps, resolves inconsistencies, and fills some of the gaps that neither of those validation suites addressed

Contains 119 benchmarks, with all of the input specifications taken from the *Handbook*

Included as a standard part of future MCNP releases from RSICC:

- Automated execution and collections of results
- Can be run with ENDF/B-VII.0, T16_2003+ENDF/B-VI, or ENDF/B-VI nuclear data libraries
- 5,000,000 neutrons per case (600 cycles, 100 cycles discarded, 10,000 neutrons per cycle)
- Run time: 7.75 hours on an 8-core Mac Pro for 714,000,000 histories

Expanded Criticality Validation Suite (2)

Principal Fuel	Number of Benchmarks by Spectrum			
	Fast	Intermediate	Thermal	Total
^{233}U	10	1	7	18
HEU	29	5	6	40
IEU	10	1	6	17
LEU			8	8
Plutonium	21	1	14	36
Total	70	8	41	119

HEU $\geq$ 60 wt.%
5 wt.% < IEU < 60 wt.%
LEU $\leq$ 5 wt.%

Fast $\geq$ 100 keV
0.625 eV < Intermediate < 100 keV
Thermal $\leq$ 0.625 eV

Expanded Criticality Validation Suite (3)

For each fuel type:

Fast benchmarks include unreflected benchmarks, benchmarks reflected by uranium, benchmarks reflected by other heavy reflectors, and benchmarks reflected by light reflectors

Except for HEU, intermediate benchmarks include whatever we could find in the *Handbook* (^{233}U benchmark is based on a substantially subcritical experiment, IEU and plutonium benchmarks are based on k_∞ measurements)

Thermal benchmarks include at least 1 reactor-type lattice and at least 2 solutions

Characteristics of ^{233}U Benchmarks

Spectrum	Form	Shape	Moderator/Reflector	Benchmark ID(s)
Fast	Metal	Sphere	Unreflected	u233-met-fast-001
			HEU	u233-met-fast-002-case-1 u233-met-fast-002-case-2
			Normal uranium	u233-met-fast-003-case-1 u233-met-fast-003-case-2 u233-met-fast-006
			Tungsten	u233-met-fast-004-case-1 u233-met-fast-004-case-2
			Beryllium	u233-met-fast-005-case-1 u233-met-fast-005-case-2
Intermediate	Solution	Sphere	Beryllium	u233-sol-inter-001-case-1
Thermal	$UO_2 + ZrO_2$	Lattice	Water	u233-comp-therm-001-case-3
	Solution	Sphere	Unreflected	u233-sol-therm-001-case-1 u233-sol-therm-001-case-2 u233-sol-therm-001-case-3 u233-sol-therm-001-case-4 u233-sol-therm-001-case-5 u233-sol-therm-008

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Characteristics of Metal HEU Spheres (1)

Spectrum	Form	Shape	Reflector	Benchmark ID(s)
Fast	Metal	Sphere	Unreflected	heu-met-fast-001 heu-met-fast-008 heu-met-fast-018-case-2
			Normal uranium	heu-met-fast-003-case-1 heu-met-fast-003-case-2 heu-met-fast-003-case-3 heu-met-fast-003-case-4 heu-met-fast-003-case-5 heu-met-fast-003-case-6 heu-met-fast-003-case-7 heu-met-fast-028
			Depleted uranium	heu-met-fast-014
			Tungsten carbide	heu-met-fast-003-case-8 heu-met-fast-003-case-9 heu-met-fast-003-case-10 heu-met-fast-003-case-11

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Characteristics of Metal HEU Spheres (2)

Spectrum	Form	Shape	Reflector	Benchmark ID(s)
Fast	Metal	Sphere	Nickel	heu-met-fast-003-case-12
			Steel	heu-met-fast-013 heu-met-fast-021-case-2
			Duralumin	heu-met-fast-022-case-2
			Aluminum	heu-met-fast-012
			Graphite	heu-met-fast-019-case-2
			Beryllium	heu-met-fast-009-case-1
			Beryllium oxide	heu-met-fast-009-case-2
			Polyethylene	heu-met-fast-011 heu-met-fast-020-case-2
			Water	heu-met-fast-004-case-1

Characteristics of Other HEU Benchmarks

Spectrum	Form	Shape	Reflector, Moderator, and/or Buffer	Benchmark ID(s)
Fast	Metal	Cylinder	Unreflected	heu-met-fast-015
		Lattice	Paraffin	heu-met-fast-026-case-c-11
Intermediate	UH_3	Cylinder	Natural uranium	heu-comp-inter-003, case-6
	Metal	Cylinder	Graphite, copper	heu-met-inter-006-case-1 heu-met-inter-006-case-2 heu-met-inter-006-case-3 heu-met-inter-006-case-4
Thermal	UO_2 + ZrO_2	Lattice	Water, ThO_2	u233-comp-therm-001-case-6
	Solution	Sphere	Unreflected	heu-sol-therm-013-case-1 heu-sol-therm-013-case-2 heu-sol-therm-013-case-3 heu-sol-therm-013-case-4 heu-sol-therm-032

Characteristics of IEU Benchmarks

Spectrum	Form	Shape	Reflector/Buffer	Benchmark(s)
Fast	Metal	Sphere	Unreflected	ieu-met-fast-003-case-2
			Steel	ieu-met-fast-005-case-2
			Duralumin	ieu-met-fast-006-case-2
			Graphite	ieu-met-fast-004-case-2
		Cylinder	Unreflected	ieu-met-fast-001-case-1 ieu-met-fast-001-case-2 ieu-met-fast-001-case-3 ieu-met-fast-001-case-4
			Normal uranium	ieu-met-fast-002
			Depleted uranium	ieu-met-fast-007-case-4
Intermediate	Plate	Lattice	Normal uranium, steel	mix-met-fast-008-case-7
Thermal	UO_2	Lattice	Water	ieu-comp-therm-002-case-3
	Solution	Cylinder	Unreflected	leu-sol-therm-007-case-14 leu-sol-therm-007-case-30 leu-sol-therm-007-case-32 leu-sol-therm-007-case-36 leu-sol-therm-007-case-49

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Characteristics of LEU Benchmarks

Spectrum	Form	Shape	Buffer/Reflector	Benchmark(s)
Thermal	UO_2	Lattice	UO_2 Rods, Water	leu-comp-therm-008-case-1 leu-comp-therm-008-case-2 leu-comp-therm-008-case-5 leu-comp-therm-008-case-7 leu-comp-therm-008-case-8 leu-comp-therm-008-case-11
	Solution	Sphere	Water	leu-sol-therm-002-case-1
			Unreflected	leu-sol-therm-002-case-2

Characteristics of Metal Plutonium Spheres

Spectrum	Form	Shape	Reflector and/or Buffer	Benchmark(s)
Fast	Metal	Sphere	Unreflected	pu-met-fast-001 pu-met-fast-002 pu-met-fast-022-case-2
			HEU	mix-met-fast-001 mix-met-fast-003
			Normal uranium	pu-met-fast-006 pu-met-fast-010
			Depleted uranium	pu-met-fast-020
			Thorium	pu-met-fast-008-case-2
			Tungsten	pu-met-fast-005
			Steel	pu-met-fast-025-case-2 pu-met-fast-026-case-2
			Aluminum	pu-met-fast-009
			Graphite	pu-met-fast-023-case-2
			Beryllium	pu-met-fast-018 pu-met-fast-019
			Polyethylene	pu-met-fast-024-case-2
			Water	pu-met-fast-011

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Characteristics of Other Plutonium Benchmarks

Spectrum	Form	Shape	Reflector/Moderator	Benchmark(s)
Fast	Metal	Cylinder	Beryllium	pu-met-fast-021-case-1
			Beryllium oxide	pu-met-fast-021-case-2
		Lattice	Unreflected	pu-met-fast-003-case-103
Intermediate	Mixture	Homog	Hydrogen, graphite	pu-comp-inter-001
Thermal	MOX	Lattice	Water	mix-comp-therm-002-case-pnl30 mix-comp-therm-002-case-pnl31 mix-comp-therm-002-case-pnl32 mix-comp-therm-002-case-pnl33 mix-comp-therm-002-case-pnl34 mix-comp-therm-002-case-pnl35
	Solution	Sphere	Unreflected	pu-sol-therm-009-case-3a pu-sol-therm-011-case-16-5 pu-sol-therm-011-case-18-1 pu-sol-therm-011-case-18-6 pu-sol-therm-021-case-1 pu-sol-therm-021-case-3
		Cylinder	Water	pu-sol-therm-018-case-9 pu-sol-therm-034-case-1

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Data Testing for ENDF/B-VII.1β3

The Expanded Criticality Suite currently is being used at Brookhaven National Laboratory and at LANL for data testing of β versions of ENDF/B-VII.1

For most criticality benchmarks, ENDF/B-VII.1β3 produces results that are in very close agreement with results from ENDF/B-VII.0

ENDF/B-VII.1β3 produces substantially improved results for cases with beryllium, tungsten, titanium, or cadmium

However, further improvement is needed for cases with beryllium

Unfortunately, a number of previously identified problems still remain, including

- Unresolved resonance range for ^{235}U
- Thermal range for ^{239}Pu
- Fast range for ^{237}Np
- Fast range for copper

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Results for Metal ^{233}U Spheres

Reflector	k_{eff}		
	Benchmark	ENDF/B-VII.1β3	ENDF/B-VII.0
None	1.0000 ± 0.0010	0.9996 ± 0.0003	0.9995 ± 0.0003
HEU	1.0000 ± 0.0010	0.9986 ± 0.0003	0.9990 ± 0.0003
HEU	1.0000 ± 0.0011	1.0002 ± 0.0003	1.0006 ± 0.0003
Normal U	1.0000 ± 0.0010	0.9990 ± 0.0003	0.9996 ± 0.0003
Normal U	1.0000 ± 0.0010	0.9993 ± 0.0003	1.0001 ± 0.0003
Normal U	1.0000 ± 0.0014	0.9987 ± 0.0003	0.9995 ± 0.0003

$\sigma < |\Delta k| \leq 2\sigma$

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Results for Metal HEU Spheres

Reflector	k_{eff}		
	Benchmark	ENDF/B-VII.1β3	ENDF/B-VII.0
None	1.0000 ± 0.0010	0.9997 ± 0.0003	0.9994 ± 0.0003
None	1.0000 ± 0.0014	0.9996 ± 0.0003	0.9999 ± 0.0003
Normal U	1.0000 ± 0.0050	0.9947 ± 0.0003	0.9948 ± 0.0003
Normal U	1.0000 ± 0.0050	0.9947 ± 0.0003	0.9945 ± 0.0003
Normal U	1.0000 ± 0.0050	0.9995 ± 0.0003	0.9991 ± 0.0003
Normal U	1.0000 ± 0.0030	0.9974 ± 0.0003	0.9971 ± 0.0003
Normal U	1.0000 ± 0.0030	1.0012 ± 0.0003	1.0008 ± 0.0003
Normal U	1.0000 ± 0.0030	1.0019 ± 0.0003	1.0020 ± 0.0003
Normal U	1.0000 ± 0.0030	1.0018 ± 0.0003	1.0018 ± 0.0003
Depleted U	0.9989 ± 0.0017	0.9976 ± 0.0003	0.9978 ± 0.0003

$\sigma < |\Delta k| \leq 2\sigma$

Results for Metal Plutonium Spheres

Reflector	k_{eff}		
	Benchmark	ENDF/B-VII.1β3	ENDF/B-VII.0
None	1.0000 ± 0.0010	1.0000 ± 0.0003	1.0000 ± 0.0003
None	1.0000 ± 0.0014	0.9998 ± 0.0003	0.9999 ± 0.0003
Normal U	1.0000 ± 0.0030	1.0002 ± 0.0003	0.9995 ± 0.0003
Normal U	1.0000 ± 0.0018	0.9998 ± 0.0003	1.0001 ± 0.0003
Depleted U	0.9993 ± 0.0017	0.9981 ± 0.0003	0.9981 ± 0.0003
Thorium	1.0000 ± 0.0006	0.9978 ± 0.0003	0.9977 ± 0.0003

$|\Delta k| > 3\sigma$

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Results for Metal Spheres Reflected by Tungsten or Tungsten Carbide

Fuel	Fuel Radius (cm)	Reflector Thickness (cm)	k_{eff}		
			Benchmark	ENDF/B-VII.1β3	ENDF/B-VII.0
^{233}U	5.0444	2.4384	1.0000 ± 0.0007	0.9987 ± 0.0003	1.0049 ± 0.0003
^{233}U	4.5999	5.7912	1.0000 ± 0.0008	0.9954 ± 0.0003	1.0052 ± 0.0003
HEU	6.6020	4.8260*	1.0000 ± 0.0050	1.0014 ± 0.0003	1.0082 ± 0.0003
HEU	6.2527	7.3660*	1.0000 ± 0.0050	1.0014 ± 0.0003	1.0095 ± 0.0003
HEU	6.0509	11.4300*	1.0000 ± 0.0050	1.0050 ± 0.0003	1.0129 ± 0.0003
HEU	6.0159	16.5100*	1.0000 ± 0.0050	1.0099 ± 0.0003	1.0166 ± 0.0003
Pu	5.0419	4.6990	1.0000 ± 0.0013	1.0011 ± 0.0003	1.0093 ± 0.0003

* Tungsten carbide reflector

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$ $3\sigma < |\Delta k|$

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Results for Metal Spheres Reflected by Beryllium or Beryllium Oxide

Fuel	Fuel Radius (cm)	Reflector Thickness (cm)	k_{eff}		
			Benchmark	ENDF/B-VII.1β3	ENDF/B-VII.0
^{233}U	5.0444	2.0447	1.0000 ± 0.0030	0.9963 ± 0.0003	0.9941 ± 0.0003
^{233}U	4.5999	4.1961	1.0000 ± 0.0030	0.9956 ± 0.0003	0.9924 ± 0.0003
HEU	8.3500	2.6500	0.9992 ± 0.0015	0.9976 ± 0.0003	0.9949 ± 0.0003
HEU	8.3500*	2.6500**	0.9992 ± 0.0015	0.9967 ± 0.0003	0.9955 ± 0.0003
Pu	5.0419	3.6881	1.0000 ± 0.0030	0.9993 ± 0.0003	0.9964 ± 0.0003
Pu	5.3500*	5.6500	0.9992 ± 0.0015	1.0009 ± 0.0003	0.9976 ± 0.0003
Pu	3.7938	8.4938	0.9983 ± 0.0019	1.0000 ± 0.0003	0.9965 ± 0.0003

* Inner radius 1.4 cm
** Beryllium oxide reflector

$\sigma < |\Delta k| \leq 2\sigma$ $2\sigma < |\Delta k| \leq 3\sigma$

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Summary

The Expanded Criticality Validation Suite provides a significant advance in the quality assurance and validation of MCNP for criticality applications

The careful selection of benchmarks from the *Handbook* that span the expected range of applicability provides the required broad coverage of criticality applications

The Expanded Criticality Suite currently is being used at Brookhaven National Laboratory and at LANL for data testing of β versions of ENDF/B-VII.1, and it is expected that it will continue to be used to assess the impact of future improvements to ENDF/B nuclear data libraries

For practitioners, the Suite may also serve as a starting point for validating MCNP and its nuclear data libraries for their specific applications