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An Expanded Criticality Validation Suite for MCNP

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INTRODUCTION

Criticality safety practitioners are required to validate the computational tools used in their work. The computer code validation effort typically involves analyzing a set of experimental benchmarks that are similar to the problem of interest and then assessing the accuracy of the computed results vs. benchmark measurements. That is, the focus is to determine whether a general-purpose tool performs adequately for a specific problem of interest. Computer code developers are faced with a different validation task, that of determining whether the code performs properly for a wide range of different possible problems.

The "correctness" of a computer code is traditionally discussed in terms of the verification and validation processes. Verification involves performing a series of calculations to determine whether a code faithfully solves the equations and physical models it was designed to solve. Verification may involve comparison to other codes, to analytic benchmarks, or to experiments. Validation involves a determination of whether the code faithfully reproduces reality for a particular range of applications of interest. Validation may involve assessing the verification problems (to ensure that end-user applications are bounded), comparing calculations to relevant experiments, or performing scoping studies (to ensure that parameter changes produce expected changes in results). While code developers can thoroughly verify their codes, validation is problematic because of the very wide range of different problems and different code options. Validation performed by code developers must necessarily be general, involving suites of problems chosen to broadly represent and span the range of possible applications.

The MCNP [1] code developers have done so using over a dozen verification/validation suites for testing general classes of problems, including regression/installation, shielding, electrons, photons, reactor kinetics parameters, variance reduction, etc. The MCNP validation suites should not be used as an absolute indicator of the accuracy or reliability of MCNP5 or the nuclear data libraries. Many of the benchmarks are taken from sequences of similar benchmarks, and the sequence as a whole may display sensitivities that a single case cannot capture. Nonetheless, the suites can provide a general indication of the overall performance of a given library, and can alert the user to unexpected or unintended consequences resulting from changes to nuclear data. In addition, the test suites can help to identify areas where improvements are needed. This paper focuses on verification/validation of MCNP5 for criticality safety and reactor applications.

PREVIOUS MCNP CRITICALITY SUITES

Two criticality validation suites for the MCNP Monte Carlo code have been used at Los Alamos National Laboratory (LANL) for nearly a decade. Those criticality validation suites were created independently by the Nuclear Data team and Monte Carlo teams. However, there is some overlap between them as well as inconsistencies. In addition, neither adequately addresses certain areas of nuclear data. Consequently, an expanded criticality validation suite [2] has been created that incorporates many of the benchmarks in those two suites, eliminates overlaps, resolves inconsistencies, and fills some of the gaps that neither of them addresses.

The nuclear data team's suite [3,4] initially included 86 separate benchmarks but eventually expanded to 93 benchmarks. The suite is used primarily for nuclear data testing. Nearly all of the benchmarks in that suite are taken from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* [5] or from the Cross Section Evaluation Working Group (CSEWG) benchmark book [6]. They include several sets of related benchmarks so that the effects of parameter variations such as enrichment, reflector thickness, or solution content can be evaluated. However, the suite contains only fast metal systems and thermal solution systems. It does not include any lattice benchmarks, any benchmarks with intermediate spectra, or any benchmarks with low enriched uranium (LEU) fuel.

The Monte Carlo team subsequently created a suite [7] of 27 criticality benchmarks to test changes to the MCNP Monte Carlo code and to its distributed nuclear data libraries. That suite eventually expanded to 31 benchmarks [8], although not all of the benchmarks in the initial version of the suite are retained in the later version. The objective was to have a wide representation of fissile materials, reflector materials, and spectra. The suite includes at least three fast, one intermediate, and two thermal benchmarks for ^{233}U systems, highly enriched uranium (HEU) systems, intermediate enriched uranium (IEU) systems, and plutonium systems. For LEU systems, it only includes thermal benchmarks, because they cannot reach criticality with intermediate or fast spectra. The three subcategories for fast systems are benchmarks that are unreflected, reflected by a heavy material, and reflected by a light material. The subcategories for thermal systems are lattice and solution benchmarks. However, the suite does not include subsets of related benchmarks that would permit parameter variations to be studied. All of the benchmarks in the Monte Carlo team's suite are taken from the *Handbook*.

EXPANDED VALIDATION SUITE

All of the benchmarks in the expanded validation suite are taken from the *Handbook*, with the exception of one benchmark (ieu-met-fast-007-case-4) that has been submitted for inclusion but has not yet been approved. The name of each benchmark is the same as the identifier for the evaluation in the *Handbook* from which it is taken. In those cases where the evaluation includes more than one case, the benchmark name appends the case number to the identifier. Reference [2] provides a complete description of the Expanded Validation Suite, with descriptions and complete MCNP input specifications for each of the problems.

The benchmarks in the expanded validation suite are divided according to the isotope that produces the majority of fissions: ^{233}U, ^{235}U, or ^{239}Pu. The ^{235}U benchmarks are further subdivided by the fractional ^{235}U content in the uranium as HEU, IEU, or LEU. HEU contains 60 wt.% or more ^{235}U, and LEU contains 5 wt.% or less. IEU therefore contains between 5 wt.% and 60 wt.% ^{235}U. The ^{239}Pu category is generalized to include all plutonium isotopes and hereafter is referred to simply as plutonium. The number of cases in the expanded validation suite in each of these categories is shown in Table I, which also indicates the degree of overlap with the benchmarks in the two previous criticality validation suites.

It should be noted that the expanded validation suite uses 5 wt.% as the dividing line between LEU and IEU, whereas the *Handbook* uses 10 wt.%. The reason that 5 wt.% was chosen is that it is the current enrichment limit for fuel used in commercial nuclear reactors in the United States.

Table I. Benchmarks in the Expanded Criticality Validation Suite

	Number of Benchmarks			
Principal Fuel	Data Team Suite	MC Team Suite	Other	Expanded Suite
U-233	12	6	-	18
HEU	30	7	3	40
IEU	7	5	5	17
LEU	-	2	6	8
Pu	19	9	8	36
Total	**68**	**29**	**22**	**119**

The expanded validation suite follows the guidelines from the *Handbook* in classifying spectra as fast, intermediate, or thermal. Fast benchmarks are those in which the majority of fissions is caused by neutrons with energy greater than 100 kev, and thermal benchmarks are those in which the majority of fissions is caused by neutrons with energies less than 0.625 eV. Benchmarks with intermediate spectra therefore are those in which the majority of fissions is caused by neutrons with energies between 0.625 eV and 100 keV. The spectral distribution of the benchmarks in the expanded validation suite is summarized in Table II.

Table II. Spectral Distribution of Benchmarks in the Expanded Criticality Validation Suite

	Number of Benchmarks			
Principal Fuel	Fast	Intermediate	Thermal	Total
U-233	10	1	7	18
HEU	29	5	6	40
IEU	10	1	6	17
LEU	-	-	8	8
Pu	21	1	14	36
Total	**70**	**8**	**41**	**119**

Tables III-IX provide a summary of the *Handbook* cases selected for the 119 problems in the Expanded Validation Suite. This collection of benchmark problems has also been transmitted to the CSEWG evaluators.

MCNP IMPLEMENTATION

The Expanded Validation Suite with 119 problems is packaged in the same fashion as other MCNP test suites, as part of the *Testing* directory in the MCNP distribution. It is currently available for both MCNP5 and MCNP6 (under development). At this writing, it is not included with the MCNP5 distribution package from RSICC; plans are to include it in the next update. Many of the problems include different input for specifying either ENDF/B-VI cross-section data, ENDF/B-VI + T16 data, or ENDF/B-VII.0 data. For some nuclides, elemental datasets are used with ENDF/B-VI data, while isotopes must be listed explicitly for ENDF/B-VII.0. For convenience, users can specify "*make ENDF=6*", "*make ENDF=16*", or "make *ENDF=7*" to instruct MCNP to use the proper problem input and cross-section libraries. Other datasets can be specified with trivial modifications to the testing *Makefile*.

The full suite of 119 problems is run using 600 cycles for each problem with 10,000 neutrons/cycle, with the first 100 cycles discarded for source convergence. Results are based on 5 M active neutron histories for each problem, giving standard deviations for k_{eff} in the range 0.0002-0.0005. For the entire suite, a total of 714 M neutron histories is run. The entire suite takes about 7 hr 45 min (wallclock) to run on a 3 GHz dual quad-core Mac Pro using 8 threads for all problems (about 60 cpu-hr total), with MCNP5-1.60 and ENDF/B-VII.0 data. For regression testing purposes, where the primary goal is to confirm code consistency and stability, a shortened version of the suite can be run in about 30 minutes.

Along with the problem input and testing *Makefile*, a *perl* script is provided to automatically collect all calculated k_{eff} and standard deviation results. The results are listed nicely, with accompanying *Handbook* reference values and flags to indicate significant differences between calculated and benchmark results.

CONCLUSIONS

The Expanded Validation Suite provides a significant advance in the quality assurance and verification/ validation of MCNP for criticality problems. The careful selection of *Handbook* benchmark problems that span the expected application space provides the required broad coverage of code applicability. For validation purposes, it is expected that the suite will be used with different cross-section libraries, e.g., ENDF/B-VII.1, to broadly assess the impact of library improvements. For practitioners, the suite may also serve as a starting point for validating MCNP and its data libraries for their specific applications.

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Table III. U-233 Benchmark Characteristics

Spectrum	Form	Shape	Moderator and /or Reflector	Benchmark(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

Table IV. HEU Benchmark Characteristics, Part I

Spectrum	Form	Shape	Reflector	Benchmark(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
			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 oxide	heu-met-fast-009-case-2
			Beryllium	heu-met-fast-009-case-1
			Polyethylene	heu-met-fast-011 heu-met-fast-020-case-2
			Water	heu-met-fast-004-case-1
		Cylinder	Unreflected	heu-met-fast-015
		Lattice	Paraffin	heu-met-fast-026-case-c-11

Table V. HEU Benchmark Characteristics, Part II

Spectrum	Form	Shape	Reflector, Moderator and/or Buffer	Benchmark(s)
Intermediate	UH_3	Cylinders	Natural uranium	heu-comp-inter-003, case-6
	Metal	Cylinders	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-inter-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

Table VI. IEU Benchmark Characteristics

Spectrum	Form	Shape	Reflector and/or 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
		Cylinders	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-027-case-14 leu-sol-therm-027-case-30 leu-sol-therm-027-case-32 leu-sol-therm-027-case-36 leu-sol-therm-027-case-49

Table VII. LEU Benchmark Characteristics

Spectrum	Form	Shape	Buffer and/or 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

Table VIII. Pu Benchmark Characteristics, Part I

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
		Cylinders	Beryllium oxide	pu-met-fast-021-case-2
			Beryllium	pu-met-fast-021-case-1
		Lattice	Unreflected	pu-met-fast-003-case-103

Table IX. Pu Benchmark Characteristics, Part II

Spectrum	Form	Shape	Reflector and/or Moderator	Benchmark(s)
Intermediate	Mixture	Homogeneous	Hydrogen, graphite	pu-comp-inter-001
Thermal	MOX	Lattice	Water	mix-comp-therm-002-case-pnl-30 mix-comp-therm-002-case-pnl-31 mix-comp-therm-002-case-pnl-32 mix-comp-therm-002-case-pnl-33 mix-comp-therm-002-case-pnl-34 mix-comp-therm-002-case-pnl-35
	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