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VERIFICATION OF MCNP5

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ABSTRACT

MCNP Version 5 (MCNP5) comprises a complete modernization of the MCNP Monte Carlo code. A key requirement for MCNP5 was to preserve all previously-existing MCNP capabilities. Four sets of verification problems were used to ensure code correctness: a suite of 42 regression tests, a suite of 26 criticality benchmark problems, a suite of 10 analytic benchmarks for criticality, and a suite of 19 radiation shielding validation problems. In nearly all problems, MCNP5 results exactly match those of MCNP4C2. The few that differ agree well within statistics. It is concluded that MCNP5 is verified to be as reliable and accurate as previous versions and that all previously-existing capabilities have been preserved.

Key Words: Monte Carlo, verification, benchmark problems

1. INTRODUCTION

MCNP [1] is a well-known and widely used Monte Carlo code for neutron, photon, and electron transport simulations. During the past 18 months, an intensive effort to modernize MCNP was carried out by the Monte Carlo Team at LANL. The result of this effort is MCNP Version 5 (MCNP5). As discussed in [2], the modernization of MCNP was undertaken to improve the software engineering practices, to ensure strict adherence to standards for Fortran-90 and parallel processing with MPI and OpenMP, and to provide increased flexibility for rapidly introducing new code features. All of these goals were met, and in addition many new features were added: plotting enhancements, photon Doppler broadening, radiography image tallies, enhancements to source definitions, improved variance reduction, improved random number generator, tallies on a superimposed mesh, edits of criticality safety parameters.

The MCNP modernization effort resulted in reworking every line of previously-existing source coding, using *perl* scripts to automate much of the conversion to Fortran-90 syntax and hands-on programmer recoding for more complex changes (e.g., dynamic allocation of Fortran-90 arrays, replacement of 96-way computed GOTOs by CASE statements, etc.). MCNP5 contains about 90K lines of Fortran-90 coding.

During this massive recoding effort, a fundamental requirement was that all previously-existing code capabilities must be preserved and no new code errors could be introduced. This requirement was inviolable, and was enforced by extensive testing throughout the entire code development effort. All previously existing code capabilities have been preserved, including physics options, geometry, tallying, plotting, cross-section handling, etc. Tally results from MCNP5 are expected to match the tally results of problems that can be run with the previous

MCNP4C2, except where bugs were discovered and fixed in the conversion process. Changes in the format and presentation of some of the printed output are allowed, but the tally results (*mctal* files) are required to match MCNP4C2 results in all installation/regression tests. All user input files that were used with previous versions should still work; no changes to input are required for using MCNP5 except to utilize new features.

The remainder of this paper focusses on the testing and verification of MCNP5. Four sets of verification problems were used to ensure code correctness: a suite of 42 regression tests, a suite of 26 criticality benchmark problems [3], a suite of 10 analytic benchmarks for criticality [4], and a suite of 19 radiation shielding validation problems [3] . In nearly all problems, MCNP5 results exactly match those of MCNP4C2. The few that differ agree well within statistics. It is concluded that MCNP5 is verified to be as reliable reliable and accurate as previous versions and that all previously-existing capabilities have been preserved.

2. DESCRIPTION OF TESTING/VERIFICATION SUITES

The "correctness" of a computer code is traditionally discussed in terms of verification and validation processes. Verification, generally performed by code developers, 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, generally performed by end-users, 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 the end-user application is bounded), comparing calculations to relevant experiments, or scoping studies (to ensure that parameter changes produce expected changes in results).

The MCNP5 developers have verified that MCNP5 produces the same results as the previous version, MCNP4C2, for a set of over 100 verification test problems. A few test problems produce results which match within statistics, but do not agree bit-for-bit; these differences are small and are attributed to computer roundoff due to the use of different compilers and the sensitivity of Monte Carlo eigenvalue calculations to roundoff. The verification problems used in this testing are grouped into 4 suites which are described below along with detailed discussion of the test results.

2.1. Regression Test Suite

For many years, the MCNP distribution has included a set of installation tests to verify that installation and compilation of the code are carried out correctly on a given computer system. For these tests, reference "templates" are provided for both the printed code output and resulting tally files (*mctal* files), and are compared with the actual output and *mctal* files. In the past, these tests took a few minutes each, so that the entire test set required ~1/2 hour or more. On today's computers, including PCs, an expanded test set of 42 problems executes in less than 5 minutes. Due to the short running time, the test set is typically run many times each day by an individual code developer and is now used for regression testing, rather than just installation testing. Today's code development process typically consists of modifying a few subroutines, incremental recompilation using GNU *make*, and then running the regression test set.

During the development of MCNP5, the regression test set was expanded from 28 to 42 problems, with new tests added to cover new code features or to explicitly test that particular bugs were fixed. Previous analysis of MCNP has indicated that the tests cover approximately 80-90% of the total lines of coding. (Test coverage analysis for MCNP5 is in progrss.) The MCNP5 build system specifically includes capabilities for running any or all of the regression tests and for comparing results with the reference templates.

It is important to note that the regression tests do not verify code correctness; they are used only for the purpose of detecting unintended changes to the code. Nevertheless, their extensive use on a daily basis serves to prevent the inadvertent introduction of bugs.

2.2. Criticality Validation Suite

The criticality validation suite [3] contains 26 cases that encompass a wide variety of fissile materials and spectra. Specifically, they include the three major fissile isotopes — ^{233}U, ^{235}U, and ^{239}Pu — in configurations that produce fast, intermediate, and thermal spectra. Furthermore, the ^{235}U cases were chosen so that they include highly enriched uranium (HEU), intermediate-enriched uranium (IEU), and low-enriched uranium (LEU) fuels.

The cases in the suite also were chosen to include a variety of configurations. The fast-spectrum cases include bare spheres, cores reflected by a heavy material (normal U), and cores reflected by a light material (Be or water). The thermal-spectrum cases include lattices of fuel pins as well as homogeneous solutions. The number of experiments with intermediate spectra is much more limited, and those cases were chosen primarily for availability rather than specific attributes.

The specifications for all 26 cases in the criticality validation suite are taken from the *International Handbook of Evaluated Criticality Benchmark Experiments* [5].The 26 cases are summarized in Table 1. All of the cases are at room temperature and pressure.

The calculations all were performed in sequential (single-processor) mode on a Silicon Graphics Origin 2000 supercomputer at Los Alamos National Laboratory. Each of the cases employed 250 generations of 5,000 neutron histories each, and the results from the first 50 generations were discarded. Consequently, the results reported herein are based on 1,000,000 active neutrons histories for each case. For each case, calculations were run with both code versions using ENDF60+URES data [6,7] and also using the newer ENDF66 data [9].

The values of k_{eff} for these 26 cases are given in Table 2. MCNP5 and MCNP4C2 produce identical answers for 49 of the 52 cases and agree within statistics for the other 3 cases. For the Zeus(2) cases, both code versions agree exactly using ENDF66 data. Using the ENDF60+URES data, the Zeus(2) cases tracked identically for 125 generations (0.625M histories), and final results agree within statistics.For the HEU-MT-003 (4) cases with the ENDF60+URES data, both codes agreed exactly. Using the ENDF66 data, the codes track for the first 225 generations (1.125M histories), and the final results agree within statistics. Similarly, the IEU-CT-002 (3) cases matched using ENDF60+URES data, and differed slightly using ENDF66 data, with final results agreeing within statistics.

Table 1. Summary of MCNP Criticality Validation Suite

	Name	Spectrum	Handbook ID	Description
1	Jezebel-233	Fast	U233-MET-FAST-001	Bare sphere of ^{233}U
2	Flattop-23	Fast	U233-MET-FAST-006	Sphere of ^{233}U reflected by normal U
3	U233-MF-005 (2)	Fast	U233-MET-FAST-005, case 2	Sphere of ^{233}U reflected by beryllium
4	Falstaff (1)	Intermediate	U233-SOL-INTER-001, case 1	Sphere of uranyl fluoride solution enriched in ^{233}U
5	ORNL-11	Thermal	U233-SOL-THERM-008	Large sphere of uranyl nitrate solution enriched in ^{233}U
6	Godiva	Fast	HEU-MET-FAST-001	Bare HEU sphere
7	Flattop-25	Fast	HEU-MET-FAST-028	HEU sphere reflected by normal U
8	Godiver	Fast	HEU-MET-FAST-004	HEU sphere reflected by water
9	HISS/HUG	Intermediate	HEU-COMP-INTER-004	Infinite, homogeneous mixture of HEU, H, and graphite
10	ZEUS (2)	Intermediate	HEU-MET-INTER-006, case2	HEU platters moderated by graphite and reflected by Cu
11	HEU-MT-003 (4)	Thermal	HEU-MET-THERM-003, case 4	Lattice of HEU cubes reflected by water
12	ORNL-10	Thermal	HEU-SOL-THERM-032	Large sphere of HEU nitrate solution
13	IEU-MF-003	Fast	IEU-MET-FAST-003	Bare sphere of IEU (36 wt.%)
14	BIG TEN	Fast	IEU-MET-FAST-007	Cylinder of IEU (10 wt.%) reflected by normal U
15	IEU-MF-004	Fast	IEU-MET-FAST-004	Sphere of IEU (36 wt.%) reflected by graphite
16	IEU-CT-002 (3)	Thermal	IEU-COMP-THERM-002, case 3	Lattice of IEU (17 wt.%) fuel rods in water
17	BAW XI (2)	Thermal	LEU-COMP-THERM-008, case 2	Large lattice of PWR fuel pins in borated water
18	SHEBA-2	Thermal	LEU-SOL-THERM-001	Cylinder of LEU fluoride solution enriched to 5 wt.%
19	Jezebel	Fast	PU-MET-FAST-001	Bare sphere of Pu
20	Jezebel-240	Fast	PU-MET-FAST-002	Bare sphere of Pu (20.1 at.% ^{240}Pu)
21	Flattop-Pu	Fast	PU-MET-FAST-006	Pu sphere reflected by normal U
22	PU-MF-011	Fast	PU-MET-FAST-011	Pu sphere reflected by water
23	Pu Buttons	Fast	PU-MET-FAST-003, case 3	3 x 3 x 3 array of small cylinders of Pu
24	HISS/HPG	Intermediate	PU-COMP-INTER-001	Infinite, homogeneous mixture of Pu, hydrogen, and graphite
25	PNL-33	Thermal	MIX-COMP-THERM-002, case 4	Lattice of mixed-oxide fuel pins in borated water
26	PNL-2	Thermal	PU-SOL-THERM-021, case 3	Sphere of plutonium nitrate solution

Table 2. K-effective for Cases in Criticality Validation Suite

	Name	K-effective Results Using ENDF60+URES Data		K-effective Results Using ENDF66 Data	
		MCNP5	MCNP4C2	MCNP5	MCNP4C2
1	Jezebel-233	0.99241 (57)	"	0.99106 (56)	"
2	Flattop-23	0.99931 (71)	"	0.99960 (72)	"
3	U233-MF-005 (2)	0.99785 (64)	"	0.99900 (59)	"
4	Falstaff (1)	0.99040 (104)	"	0.99017 (106)	"
5	ORNL-11	0.99596 (41)	"	0.99708 (37)	"
6	Godiva	0.99728 (63)	"	0.99647 (60)	"
7	Flattop-25	0.99790 (63)	"	0.99660 (59)	"
8	Godiver	0.99539 (80)	"	0.99675 (79)	"
9	HISS/HUG	1.01264 (47)	"	1.01016 (46)	"
10	ZEUS (2)	0.99722 (73)	0.99655 (71)	0.99538 (75)	"
11	HEU-MT-003 (4)	0.98257 (88)	"	0.98413 (79)	0.98374 (80)
12	ORNL-10	0.99874 (39)	"	0.99835 (40)	"
13	IEU-MF-003	1.00046 (57)	"	0.99973 (61)	"
14	BIG TEN	1.00987 (55)	"	1.00725 (54)	"
15	IEU-MF-004	1.00381 (62)	"	1.00315 (67)	"
16	IEU-CT-002 (3)	1.00024 (70)	"	1.00029 (74)	0.99987 (71)
17	BAW XI (2)	0.99837 (60)	"	0.99863 (70)	"
18	SHEBA-2	1.01064 (77)	"	1.01018 (82)	"
19	Jezebel	0.99694 (57)	"	0.99772 (60)	"
20	Jezebel-240	0.99883 (60)	"	0.99884 (57)	"
21	Flattop-Pu	1.00138 (66)	"	1.00266 (70)	"
22	PU-MF-011	0.99736 (76)	"	0.99700 (72)	"
23	Pu Buttons	0.99581 (67)	"	0.99735 (68)	"
24	HISS/HPG	1.01126 (59)	"	1.00936 (56)	"
25	PNL-33	1.00578 (79)	"	1.00545 (80)	"
26	PNL-2	1.00031 (104)	"	1.00219 (95)	"
	Notes:	" = result identical to that of column at left (NN) = std deviation is NN x 10^{-5}			

The statistically insignificant differences observed in 3 of the 52 cases are attributed to roundoff associated with compiler differences. The MCNP4C2 code was compiled approximately 2 years previously using a Fortran-77 compiler and associated math libraries; the MCNP5 code was compiled using the current version of the SGI Fortran-90 compiler and associated libraries. In addition, Monte Carlo eigenvalue calculations are very sensitive to computer roundoff due to their iterative nature – small differences in even a single particle history will propagate through all future generations. (Fixed source calculations are less sensitive to roundoff, since generations are not used; roundoff differences affect only a single history and do not propagate.)

Table 3. Results for Analytic Criticality Benchmarks

	Name	Description	Exact K-eff	MCNP5 K-eff
1	Ua-1-0-IN	Infinite medium, 1 group	2.25	2.24996 (24)
2	Ua-1-0-SP	Sphere, 1 group	1.0	0.99990 (23)
3	Uc-H2O(2)-1-0-SP	Reflected sphere, 1 group	1.0	0.99985 (23)
4	UD2O-1-0-CY	Cylinder, 1 group	1.0	0.99996 (15)
5	PUa-1-1-SL	Slab, 1 grp, P1 scatter	1.0	0.99989 (26)
6	UD2OB-1-1-SP	Sphere, 1 grp, P1 scatter	1.0	0.99993 (17)
7	PU-2-0-IN	Infinite medium, 2 group	2.683767	2.68375 (7)
8	URRa-2-0-SL	Slab, 2 group	1.0	1.00001 (34)
9	URR-6-0-IN	Infinite medium, 6 group	1.60	1.59999 (2)
10	URRd-H2O(1)2-0-ISLC	Slab, 2 group	1.0	0.99986 (41)
		Note: (NN) = std deviation is NN x 10^{-5}		

2.3. Analytic Benchmarks for Criticality

Reference [4] provides a set of 75 criticality problems found in the literature for which exact analytical solutions are known. Number densities, geometry, and cross-section data are specified exactly for these problems. As part of the MCNP5 verification, 10 of these analytic benchmark problems were run to high precision using MCNP5 on 2 different computer systems - a Silicon Graphics Origin 2000 supercomputer and a Pentium-III PC running Windows-2000. The 10 cases selected from [4] are listed in Table 3 along with both the analytic results and the MCNP5 results. For all cases, a total of 210 generations were run, with the first 10 discarded for settling. For cases 1-9, 40,000 histories were used per generation, for a total of 8M histories in the 200 active cycles. For case 10, only 5,000 histories per generation were run, for a total of 1M histories in the active generations. In all cases, MCNP5 results were identical on the SGI system and PC, and all results were in statistical agreement with the exact k-effective values.

2.4. Radiation Shielding Validation Suite

The radiation-shielding validation suite [3] contains three subcategories: time-of-flight spectra for neutrons from pulsed spheres, neutron and photon spectra at shield walls within a simulated fusion reactor, and photon dose rates. Two of the cases are coupled neutron-photon calculations, while the others are exclusively neutron or exclusively photon calculations.

The time-of-flight cases are a subset of the pulsed-sphere experiments that were performed at Lawrence Livermore National Laboratory from the late 1960s into the 1980s [10-12]. The objective of these experiments was to measure the neutron emission spectrum from a variety of materials bombarded by 14 MeV neutrons. These cases in the suite are summarized in Table 4.

Table 4. Summary of MCNP Radiation Shielding Validation Suite: Pulsed Spheres

Target Material	Target Configuration	Thickness (mfp)	Detector Type	Detector Angle
Beryllium	Bare Sphere	0.8	Pilot B	30E
Carbon	Bare Sphere	2.9	NE 213	30E
Concrete	Bare Sphere	2.0	NE 213	120E
Iron	Bare Sphere	0.9	NE 213	30E
Lead	Clad Sphere	1.4	NE 213	30E
^{6}Li	Dewar	1.6	NE 213	30E
Nitrogen	Dewar	3.1	Pilot B	30E
Water	Dewar	1.9	Pilot B	30E

The second subset of cases in the radiation-shielding validation suite is based on a series of experiments that was performed at Oak Ridge National Laboratory in 1980 [13]. The objective of the experiments was to simulate the deuterium-tritium neutron spectrum that would exist at the first wall of a fusion reactor as well as the spectrum of secondary photons that would be produced from neutron interactions within that wall. The fusion-shielding cases in the radiation-shielding validation suite are summarized in Table 5. The last column indicates whether the detector was aligned with the axis of the particle beam.

Table 5. Summary of MCNP Radiation Shielding Validation Suite: Fusion Shielding

Configuration	Tally Type	On/Off Axis
1	neutron	On
3	neutron	Off
3	photon	On
7	neutron	On
7	photon	Off

The cases in the last subset of the radiation-shielding validation suite are based on experimental measurements of photon dose rates. The first case is based on a 1980 measurement of air-scattered photon radiation far from the source ("skyshine") [14]. The second case is an idealization of a number of measurements of the radiation environment in an open field covered by fallout [15]. The remaining four cases model some of the Hupmobile thermoluminescent dosimeter (TLD) experiments performed at Lawrence Berkeley Laboratory between 1967 and 1969 [16,17]. The six cases are summarized in Table 6.

Table 6. Summary of MCNP Radiation Shielding Validation Suite: Photon Dose Rates

Case	Source	Principal Media
Skyshine	^{60}Co	Air and Soil
Air over Ground	^{60}Co	Air and Soil
^{60}Co through Air	^{60}Co	Air
^{60}Co through Teflon	^{60}Co	Teflon
Sm K_{α} through Air	Sm K_{α}	Air
Sm K_{α} through Teflon	Sm K_{α}	Teflon

The MCNP calculations for the cases in this suite that include photons use the MCPLIB02 photon data library [8] for all nuclides. MCPLIB02 was part of the ENDF60 library release, but it is not based on ENDF/B-VI. Instead, it is an extension of the original MCPLIB photon library that has been used with MCNP for more than 20 years. Specifically, it extends the range of data for photon interactions up to 100 GeV, based on the Lawrence Livermore National Laboratory Evaluated Photon Data Library [18].

The calculations for the radiation-shielding validation suite all were performed in sequential mode on a Silicon Graphics Origin 2000 supercomputer. Each case employed 1,000,000 particle histories.

The values to be considered for validation of these cases are obtained from tallies. Furthermore, the tally values are intermediate rather than final parameters, and they have to be processed and/or combined to obtain those final values. However, if the tallies from two different versions of MCNP match, the final values necessarily will match as well.

MCNP5 produces exactly the same tally values as MCNP4C2 for all the cases in the validation suite listed in Tables 4-6, given the same data library. This is true for both the older ENDF60 data and the new ENDF66 data.

3. CONCLUSIONS

We have demonstrated by extensive verification testing that MCNP5 produces results which are as reliable and accurate as the previous version, MCNP4C2. In nearly all cases, results from MCNP5 are in exact agreement with results from MCNP4C2. For a few cases involving eigenvalue calculations (which are sensitive to computer roundoff), MCNP5 and MCNP4C2 results did not match exactly, but did agree within small statistics. For fixed-source calculations (which are not sensitive to computer roundoff), all MCNP5 and MCNP4C2 results matched exactly.

As a result of the excellent agreement found in all cases run, we conclude that all of the previous verification/validation efforts carried out in support of MCNP should carry over to the present version, MCNP5. We do not presume to declare MCNP5 as validated for any particular end-user application (that is the perogative of the end-users, for their specific requirements and applications of the code), but suggest that such validation should be straightforward given the results reported herein for the MCNP5 verification testing.

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