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Title: Verification of MCNP5 - Version 1.50

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Monte Carlo Codes, X3-MCC
Los Alamos National Laboratory

1. Introduction

The latest release of the MCNP5 [1] Monte Carlo code is designated MCNP5-1.50. To verify that the code is performing correctly, several suites of verification/validation problems have been run, including:

- the "Criticality Validation Suite" [2] consisting of 31 problems from the *International Handbook of Evaluated Criticality Benchmark Experiments* [3],
- 10 problems from the suite of analytical criticality verification benchmarks [4], and
- the "Radiation Shielding Validation Suite" [5] of problems.

The Criticality Validation Suite was run with both ENDF/B-VI and ENDF/B-VII nuclear datasets. All calculations were run on Mac OS X, Linux, and Windows computing systems. Results from these calculations have been compared to results from the previous, verified version of MCNP5 (Version 1.40) and to known analytical results.

It should be noted that one of the major new features included in MCNP5-1.50 is Pulse Height Tally Variance Reduction (PHTVR). The new PHTVR features have been tested extensively and are documented separately in several references included with the MCNP5-1.50 release documentation [8, 9, 10, 11].

2. The MCNP5 Criticality Validation Suite

The MCNP criticality validation suite is a collection of 31 benchmarks taken from the *International Handbook of Evaluated Criticality Benchmark Experiments*. It contains cases for a variety of fuels, including ^{233}U, highly enriched uranium (HEU), intermediate-enriched uranium (IEU), low-enriched uranium (LEU), and plutonium. For each fuel type, there are cases with a variety of moderators, reflectors, spectra, and geometries. All of the cases are at room temperature and pressure. The cases in the suite are summarized in Table I.

The 31 benchmark problems shown in Table 1 were run using both MCNP5-1.50 and the previously-released version MCNP5-1.40, using both the previous MCNP Data Libraries (ENDF/B-VI, T16, SAB2002) and the new ENDF/B-VII libraries. All calculations were performed with 250 generations of 5,000 neutrons each, and the results from the first 50 generations were discarded. Consequently, the results for each case are based on 1,000,000 active neutron histories.

Table I. MCNP Criticality Validation Suite.

Spectrum	Fast			Intermediate	Thermal	
Geometry	Bare	Heavy Reflector	Light Reflector	Any	Lattice of Fuel Pins in Water	Solution
^{233}U	Jezebel-233	Flattop-23	U233-MF-05 (2)*	Falstaff (1)†	SB-2½	ORNL-11
HEU	Godiva Tinkertoy-2 (c-11)	Flattop-25	Godiver	UH_3 (6) Zeus (2)	SB-5	ORNL-10
IEU	IEU-MF-03	BIG TEN	IEU-MF-04	Zebra-8H‡	IEU-CT-02 (3)	STACY-36
LEU					BaW XI (2)	LEU-ST-02 (2)
Pu	Jezebel Jezebel-240 Pu Buttons (3)	Flattop-Pu THOR	Pu-MF-11	HISS/HPG‡	PNL-33	PNL-2

* Numbers in parentheses identify a specific case within a sequence of benchmarks
† Extrapolated to critical
‡ k_∞ measurement

A. Compiler Options and the Criticality Validation Suite

Previous versions of MCNP5 were compiled using different compiler options for different combinations of Fortran-90 compiler and computer system. For example, the *-r8* Fortran-90 compile option was used with compilers on Linux systems, but was not used on Mac OS X or Windows systems. This option converts (at compile time) all single-precision constants into their double-precision equivalents. That is, the Fortran-90 statements

```
real(8) x
x = .3
```

are converted at compile time to the statements

```
real(8)  x
x = .3d0
```

To a novice Fortran programmer, these 2 sets of statements may appear equivalent. For Monte Carlo calculations, however, the difference between the 2 sets can lead to roundoff differences in computer arithmetic (note: differences, not errors) due to the different precision of .3 as a single precision value and .3d0 as a double-precision value. If the first set of statements is compiled without the *-r8* option and the value of x is printed, and then compiled with the *-r8* option and the value of x is printed, these results are seen (on Mac OS X with the Intel Fortran-90 compiler):

Without *-r8*: x = 0.3000000119209290
With *-r8* x = 0.3000000000000000

While the relative error between the 2 results is only $4x10^{-8}$, such differences in numerical precision can lead to different particle tracking and collision analysis results in MCNP5 calculations. Because the number of accurate digits in the physical data (cross-sections) can be counted on one hand, computer roundoff differences as shown above have no physical significance, and any particle tracking differences caused by such roundoff are <u>not</u> errors in the code or data. Tracking differences due to computer roundoff do, however, complicate the verification and validation process. In an attempt to reduce the computer roundoff differences between different compilers and systems (e.g., Intel F90 on Mac OS X vs Linux, Intel F90 vs Absoft F90 on Mac OS X, etc.), we deliberately chose to use the *-r8* compiler option for <u>all</u> systems and compilers in the release of MCNP5-1.50.

Table 2 provides results for the Criticality Suite from MCNP5-1.40 and MCNP5-1.50, each compiled on Mac OS X with the Intel 10 compiler, both with and without the *-r8* option. It can be seen that:

- The results in Columns A and B show that both versions give identical results when compiled <u>without</u> the *-r8* option.

- Likewise, the results in Columns C and D show that both versions give identical results when compiled <u>with</u> the *-r8* option.

- Finally, comparing A/B with C/D shows that roundoff differences in results due to the *-r8* option are small, and that A/B and C/D agree within statistics. In Table 2, results that differ as a result of using or not using the *–r8* option are highlighted in yellow.

To summarize, Table 2 provides evidence that MCNP5-1.40 and the new MCNP5-1.50 produce identical results for criticality problems when consistent options are used in compiling the codes, assuming that identical inputs and data libraries are used. Furthermore, Table 2 also provides evidence that the effect of using the *-r8* compiler option is to introduce some minor differences (within statistics) for criticality problems that are due to computer roundoff differences, not to code errors.

B. Results for Criticality Validation Suite Using ENDF/B-VI Data

The 31 problems in the Criticality Validation Suite were run using both MCNP5-1.40 and MCNP5-1.50 with ENDF/B-VI nuclear data. Table 2 shows the results from calculations on a Mac Pro (2 quad-core Intel Xeon cpus, Mac OS X 10.4.11, Intel Fortran-90 compiler 10). The results for each set of runs are identical. In the discussion below, we will consider Columns C and D of Table 2, that provide results for both code versions compiled with the *-r8* F90 compiler option. The overall RMS difference between experimental and calculated results is 0.55%.

On a Mac Pro (Intel-based Mac):

- Columns C and D of Table 2 clearly demonstrate that MCNP5-1.40 and MCNP5-1.50 produce identical results when compiled with the same compiler and the same compiler options, when both versions use the ENDF/B-VI nuclear data.

- The results in Table 2 were generated from an executable compiled with Intel Fortran-90 and run using 8 threads (“tasks 8”). When the problems were rerun using only 1 thread, results were identical to those in Table 2. Additionally, results from the threaded version exactly matched the sequential (unthreaded) version. This verifies that the MCNP5 threading using OpenMP works correctly.

- When MCNP5 was recompiled with the Intel compiler to use both OpenMPI (message-passing) and OpenMP (threading), and then run using 4 MPI tasks with 2 threads each, the results were identical to those shown in Table 2. This verifies that both message-passing parallelism and threaded parallelism work correctly, when used separately and when used together.

- When MCNP5 was recompiled with the Absoft 10.1 Fortran-90 compiler (with MPI but without threading), results using 8 MPI processes were identical to those shown in Table 2 for 26 of the 31 cases, and agreed within statistics for the other 5 cases. This indicates small differences in roundoff between the executables compiled with Intel vs Absoft Fortran-90.

- When MCNP5 was recompiled with the Absoft 10.1 Fortran-90 compiler (without MPI and without threading), results using 1 processor were identical to those shown in Table 2 for 26 of the 31 cases, and agreed within statistics for the other 5 cases. These results using 1 processor exactly matched the results with Absoft using 8 MPI processes.

Table 2 Criticality Suite Results for MCNP5-1.40 and MCNP5-1.50 Using ENDF/B-VI + T16 Data Comparison without -r8 and with -r8 F90 Compile Option

			A		B		C		D	
	Experiment		mcnp5-1.40 ENDF/B-VI + T16 without -r8		mcnp5-1.50 ENDF/B-VI + T16 without -r8		mcnp5-1.40 ENDF/B-VI + T16 with -r8		mcnp5-1.50 ENDF/B-VI + T16 with -r8	
case	Keff	std dev	Keff	std dev	Keff	std dev	Keff	std dev	Keff	std dev
U233 Benchmarks										
JEZ233	1.0000	0.0010	0.9911	0.0006	0.9911	0.0006	0.9911	0.0006	0.9911	0.0006
FLAT23	1.0000	0.0014	0.9993	0.0007	0.9993	0.0007	0.9996	0.0007	0.9996	0.0007
UMF5C2	1.0000	0.0030	0.9970	0.0007	0.9970	0.0007	0.9975	0.0007	0.9975	0.0007
FLSTF1	1.0000	0.0083	0.9897	0.0011	0.9897	0.0011	0.9898	0.0010	0.9898	0.0010
SB25	1.0000	0.0024	0.9958	0.0011	0.9958	0.0011	0.9953	0.0011	0.9953	0.0011
ORNL11	1.0006	0.0029	0.9978	0.0004	0.9978	0.0004	0.9978	0.0004	0.9978	0.0004
HEU Benchmarks										
GODIVA	1.0000	0.0010	0.9968	0.0006	0.9968	0.0006	0.9968	0.0006	0.9968	0.0006
TT2C11	1.0000	0.0038	0.9976	0.0008	0.9976	0.0008	0.9976	0.0008	0.9976	0.0008
FLAT25	1.0000	0.0030	1.0028	0.0006	1.0028	0.0006	1.0025	0.0006	1.0025	0.0006
GODIVR	0.9985	0.0011	0.9940	0.0008	0.9940	0.0008	0.9947	0.0008	0.9947	0.0008
UH3C6	1.0000	0.0047	0.9921	0.0008	0.9921	0.0008	0.9921	0.0008	0.9921	0.0008
ZEUS2	0.9997	0.0008	0.9934	0.0008	0.9934	0.0008	0.9934	0.0008	0.9934	0.0008
SB5RN3	1.0015	0.0028	0.9945	0.0013	0.9945	0.0013	0.9955	0.0014	0.9955	0.0014
ORNL10	1.0015	0.0026	0.9996	0.0004	0.9996	0.0004	0.9996	0.0004	0.9996	0.0004
IEU Benchmarks										
IMF03	1.0000	0.0017	0.9990	0.0006	0.9990	0.0006	0.9986	0.0006	0.9986	0.0006
BIGTEN	0.9948	0.0013	1.0072	0.0005	1.0072	0.0005	1.0072	0.0005	1.0072	0.0005
IMF04	1.0000	0.0030	1.0039	0.0006	1.0039	0.0006	1.0035	0.0006	1.0035	0.0006
ZEBR8H	1.0300	0.0025	1.0402	0.0006	1.0402	0.0006	1.0402	0.0006	1.0402	0.0006
ICT2C3	1.0017	0.0044	0.9996	0.0007	0.9998	0.0006	1.0007	0.0007	1.0007	0.0007
STACY36	0.9988	0.0013	0.9989	0.0007	0.9989	0.0007	0.9989	0.0007	0.9989	0.0007
LEU Benchmarks										
BAWXI2	1.0007	0.0012	0.9963	0.0007	0.9963	0.0007	0.9975	0.0007	0.9975	0.0007
LST2C2	1.0024	0.0037	0.9958	0.0006	0.9958	0.0006	0.9958	0.0006	0.9958	0.0006
Pu Benchmarks										
JEZPU	1.0000	0.0020	0.9977	0.0006	0.9977	0.0006	0.9977	0.0006	0.9977	0.0006
JEZ240	1.0000	0.0020	0.9988	0.0006	0.9988	0.0006	0.9988	0.0006	0.9988	0.0006
PUBTNS	1.0000	0.0030	0.9969	0.0006	0.9969	0.0006	0.9969	0.0006	0.9969	0.0006
FLATPU	1.0000	0.0030	1.0019	0.0007	1.0019	0.0007	1.0027	0.0007	1.0027	0.0007
THOR	1.0000	0.0006	1.0054	0.0006	1.0054	0.0006	1.0054	0.0006	1.0054	0.0006
PUSH2O	1.0000	0.0010	0.9961	0.0008	0.9961	0.0008	0.9956	0.0008	0.9956	0.0008
HISHPG	1.0000	0.0110	1.0106	0.0006	1.0106	0.0006	1.0105	0.0005	1.0105	0.0005
PNL2	1.0000	0.0065	1.0035	0.0009	1.0035	0.0009	1.0035	0.0009	1.0035	0.0009
PNL33	1.0024	0.0021	1.0044	0.0007	1.0044	0.0007	1.0044	0.0007	1.0044	0.0007

black:	diff < 1 sig
blue:	1 sig < diff < 2 sig
red:	2 sig < diff

A,B,C,D std MCNP libraries, ENDF/B-VI + T16 + SAB2002
A mcnp5-1.40, compiled WITHOUT -r8 option
B mcnp5-1.50, compiled WITHOUT -r8 option
C mcnp5-1.40, compiled WITH -r8 option
D mcnp5-1.50, compiled WITH -r8 option

Table 3 **Criticality Suite Results for MCNP5-1.50 Using ENDF/B-VI + T16 Data**

	Mac OS X		Windows		Windows		Windows		Windows		Windows		Windows	
	Intel 10		Intel 9		Intel 10		Absoft 9		Absoft 10		g95		Portland	
case	Keff	std dev	Keff	std dev	Keff	std dev	Keff	std dev	Keff	std dev	Keff	std dev	Keff	std dev
U233 Benchmarks														
JEZ233	0.9911	0.0006	0.9911	0.0006	0.9911	0.0006	0.9911	0.0006	0.9911	0.0006	0.9911	0.0006	0.9911	0.0006
FLAT23	0.9996	0.0007	0.9996	0.0007	0.9996	0.0007	0.9993	0.0007	0.9993	0.0007	0.9996	0.0007	0.9996	0.0007
UMF5C2	0.9975	0.0007	0.9975	0.0007	0.9975	0.0007	0.9970	0.0007	0.9970	0.0007	0.9975	0.0007	0.9975	0.0007
FLSTF1	0.9898	0.001	0.9898	0.0010	0.9898	0.0010	0.9897	0.0011	0.9897	0.0011	0.9898	0.0010	0.9898	0.0010
SB25	0.9953	0.0011	0.9953	0.0011	0.9953	0.0011	0.9958	0.0011	0.9958	0.0011	0.9983	0.0010	0.9953	0.0011
ORNL11	0.9978	0.0004	0.9978	0.0004	0.9978	0.0004	0.9978	0.0004	0.9978	0.0004	0.9978	0.0004	0.9978	0.0004
HEU Benchmarks														
GODIVA	0.9968	0.0006	0.9968	0.0006	0.9968	0.0006	0.9968	0.0006	0.9968	0.0006	0.9968	0.0006	0.9968	0.0006
TT2C11	0.9976	0.0008	0.9979	0.0008	0.9979	0.0008	0.9978	0.0008	0.9972	0.0008	0.9975	0.0007	0.9972	0.0008
FLAT25	1.0025	0.0006	1.0025	0.0006	1.0025	0.0006	1.0028	0.0006	1.0028	0.0006	1.0025	0.0006	1.0025	0.0006
GODIVR	0.9947	0.0008	0.9947	0.0008	0.9947	0.0008	0.9940	0.0008	0.9940	0.0008	0.9947	0.0008	0.9947	0.0008
UH3C6	0.9921	0.0008	0.9921	0.0008	0.9921	0.0008	0.9921	0.0008	0.9921	0.0008	0.9913	0.0007	0.9921	0.0008
ZEUS2	0.9934	0.0008	0.9934	0.0008	0.9934	0.0008	0.9941	0.0007	0.9949	0.0008	0.9946	0.0007	0.9949	0.0008
SB5RN3	0.9955	0.0014	0.9955	0.0014	0.9955	0.0014	0.9945	0.0013	0.9945	0.0013	0.9945	0.0014	0.9955	0.0014
ORNL10	0.9996	0.0004	0.9996	0.0004	0.9996	0.0004	0.9996	0.0004	0.9996	0.0004	0.9996	0.0004	0.9996	0.0004
IEU Benchmarks														
IMF03	0.9986	0.0006	0.9986	0.0006	0.9986	0.0006	0.9990	0.0006	0.9990	0.0006	0.9986	0.0006	0.9986	0.0006
BIGTEN	1.0072	0.0005	1.0072	0.0005	1.0072	0.0005	1.0072	0.0005	1.0072	0.0005	1.0072	0.0005	1.0072	0.0005
IMF04	1.0035	0.0006	1.0035	0.0006	1.0035	0.0006	1.0039	0.0006	1.0039	0.0006	1.0035	0.0006	1.0035	0.0006
ZEBR8H	1.0402	0.0006	1.0406	0.0006	1.0406	0.0006	1.0410	0.0006	1.0401	0.0006	1.0408	0.0006	1.0397	0.0007
ICT2C3	1.0007	0.0007	1.0007	0.0007	1.0007	0.0007	1.0001	0.0006	1.0002	0.0007	0.9998	0.0007	1.0003	0.0007
STACY36	0.9989	0.0007	0.9989	0.0007	0.9989	0.0007	0.9989	0.0007	0.9989	0.0007	0.9989	0.0007	0.9989	0.0007
LEU Benchmarks														
BAWXI2	0.9975	0.0007	0.9975	0.0007	0.9975	0.0007	0.9963	0.0007	0.9963	0.0007	0.9975	0.0007	0.9975	0.0007
LST2C2	0.9958	0.0006	0.9958	0.0006	0.9958	0.0006	0.9958	0.0006	0.9958	0.0006	0.9958	0.0006	0.9958	0.0006
Pu Benchmarks														
JEZPU	0.9977	0.0006	0.9977	0.0006	0.9977	0.0006	0.9977	0.0006	0.9977	0.0006	0.9977	0.0006	0.9977	0.0006
JEZ240	0.9988	0.0006	0.9988	0.0006	0.9988	0.0006	0.9988	0.0006	0.9988	0.0006	0.9988	0.0006	0.9988	0.0006
PUBTNS	0.9969	0.0006	0.9969	0.0006	0.9969	0.0006	0.9969	0.0006	0.9969	0.0006	0.9969	0.0006	0.9969	0.0006
FLATPU	1.0027	0.0007	1.0027	0.0007	1.0027	0.0007	1.0019	0.0007	1.0019	0.0007	1.0027	0.0007	1.0027	0.0007
THOR	1.0054	0.0006	1.0054	0.0006	1.0054	0.0006	1.0054	0.0006	1.0054	0.0006	1.0054	0.0006	1.0054	0.0006
PUSH2O	0.9956	0.0008	0.9956	0.0008	0.9956	0.0008	0.9961	0.0008	0.9961	0.0008	0.9956	0.0008	0.9956	0.0008
HISHPG	1.0105	0.0005	1.0108	0.0006	1.0108	0.0006	1.0108	0.0005	1.0103	0.0005	1.0110	0.0006	1.0105	0.0006
PNL2	1.0035	0.0009	1.0035	0.0009	1.0035	0.0009	1.0035	0.0009	1.0035	0.0009	1.0035	0.0009	1.0035	0.0009
PNL33	1.0044	0.0007	1.0044	0.0007	1.0044	0.0007	1.0044	0.0007	1.0044	0.0007	1.0023	0.0008	1.0044	0.0007

shaded results differ from Mac OS X + Intel 10

The 31 problems were also run with a variety of Fortran-90 compilers on Windows and Linux. A comparison between the Mac OS X results from MCNP5-1.50 and the Windows results is shown in Table 3. In Table 3, Windows results that differ from the Mac OS X results are highlighted in yellow. It can be seen that using the Intel and Portland compilers on Windows produce results that are nearly identical to the Mac results, with only very small roundoff differences in 3 or 4 cases. The Windows g95 compiler produces differences from the Intel compilers in 9 cases, with 7 of those agreeing within 1 combined standard deviation, and the other 2 agreeing within 2 combined standard deviations. The Windows Absoft compilers produce differences in 17 cases, with all 17 agreeing within 1 combined standard deviation. None of the observed differences is significant, given the statistics on the results. It can be concluded that using different compilers can result in small differences due to arithmetic roundoff, but that the differences are small and within statistics.

On Windows (3.2GHz Pentium 4 HT, Windows XP):

- The 31 problems were run with ENDF/B-VI data using MCNP5-1.50 on a Windows platform, with 6 Fortran-90 compilers – Intel 9, Intel 10, Absoft 9, Absoft 10, g95, and Portland.

- For all of the compilers on Windows, many of the results matched the Mac results exactly. With the exception of the g95 compiler, all of the Windows results matched the Mac results within 1 combined standard deviation. For the g95 Windows compiler, 2 of the results differed from the Mac by more than 1 but less than 2 combined standard deviations.

C. Results for Criticality Validation Suite Using ENDF/B-VII Data

The 31 problems were run using both MCNP5-1.40 (compiled with the *–r8* option) and MCNP5-1.50 with both ENDF/B-VI nuclear data and ENDF/B-VII nuclear data. Table 4 shows the results from calculations on a Mac Pro (2 quad-core Intel Xeon cpus, Mac OS X 10.4.11, Intel Fortran-90 compiler 10). The results for each set of runs are identical. The overall RMS difference between experimental and calculated results is 0.50%. The agreement between experiment and calculation is clearly better for calculations run with the new ENDF/B-VII data, compared to the older ENDF/B-VI data.

Table 4 Criticality Suite Results for MCNP5-1.40 and MCNP5-1.50, Comparison of ENDF/B-VI+T16 Data and ENDF/B-VII Data

			A		B		H		I	
	Experiment		mcnp5-1.40 E6 1/10/08		mcnp5-1.50 E6 1/10/08		mcnp5-1.40, -r8 E7 + E7sab 5/13/08		mcnp5-1.50 E7 + E7sab 5/13/08	
case	Keff	std dev	Keff	std dev	Keff	std dev	Keff	std dev	Keff	std dev
U233 Benchmarks										
JEZ233	1.0000	0.0010	0.9911	0.0006	0.9911	0.0006	0.9989	0.0006	0.9989	0.0006
FLAT23	1.0000	0.0014	0.9993	0.0007	0.9993	0.0007	0.9990	0.0007	0.9990	0.0007
UMF5C2	1.0000	0.0030	0.9970	0.0007	0.9970	0.0007	0.9931	0.0006	0.9931	0.0006
FLSTF1	1.0000	0.0083	0.9897	0.0011	0.9897	0.0011	0.9861	0.0011	0.9861	0.0011
SB25	1.0000	0.0024	0.9958	0.0011	0.9958	0.0011	1.0005	0.0010	1.0005	0.0010
ORNL11	1.0006	0.0029	0.9978	0.0004	0.9978	0.0004	1.0010	0.0004	1.0010	0.0004
HEU Benchmarks										
GODIVA	1.0000	0.0010	0.9968	0.0006	0.9968	0.0006	0.9995	0.0006	0.9995	0.0006
TT2C11	1.0000	0.0038	0.9976	0.0008	0.9976	0.0008	0.9997	0.0008	0.9997	0.0008
FLAT25	1.0000	0.0030	1.0028	0.0006	1.0028	0.0006	1.0034	0.0007	1.0034	0.0007
GODIVR	0.9985	0.0011	0.9940	0.0008	0.9940	0.0008	0.9997	0.0008	0.9997	0.0008
UH3C6	1.0000	0.0047	0.9921	0.0008	0.9921	0.0008	0.9950	0.0008	0.9950	0.0008
ZEUS2	0.9997	0.0008	0.9934	0.0008	0.9934	0.0008	0.9956	0.0008	0.9956	0.0008
SB5RN3	1.0015	0.0028	0.9945	0.0013	0.9945	0.0013	0.9955	0.0013	0.9955	0.0013
ORNL10	1.0015	0.0026	0.9996	0.0004	0.9996	0.0004	0.9995	0.0004	0.9995	0.0004
IEU Benchmarks										
IMF03	1.0000	0.0017	0.9990	0.0006	0.9990	0.0006	1.0029	0.0006	1.0029	0.0006
BIGTEN	0.9948	0.0013	1.0072	0.0005	1.0072	0.0005	0.9945	0.0005	0.9945	0.0005
IMF04	1.0000	0.0030	1.0039	0.0006	1.0039	0.0006	1.0067	0.0006	1.0067	0.0006
ZEBR8H	1.0300	0.0025	1.0402	0.0006	1.0402	0.0006	1.0192	0.0006	1.0192	0.0006
ICT2C3	1.0017	0.0044	0.9996	0.0007	0.9998	0.0006	1.0035	0.0008	1.0035	0.0008
STACY36	0.9988	0.0013	0.9989	0.0007	0.9989	0.0007	0.9994	0.0006	0.9994	0.0006
LEU Benchmarks										
BAWXI2	1.0007	0.0012	0.9963	0.0007	0.9963	0.0007	1.0022	0.0007	1.0022	0.0007
LST2C2	1.0024	0.0037	0.9958	0.0006	0.9958	0.0006	0.9940	0.0006	0.9940	0.0006
Pu Benchmarks										
JEZPU	1.0000	0.0020	0.9977	0.0006	0.9977	0.0006	0.9993	0.0007	0.9993	0.0007
JEZ240	1.0000	0.0020	0.9988	0.0006	0.9988	0.0006	0.9992	0.0005	0.9992	0.0005
PUBTNS	1.0000	0.0030	0.9969	0.0006	0.9969	0.0006	0.9996	0.0006	0.9996	0.0006
FLATPU	1.0000	0.0030	1.0019	0.0007	1.0019	0.0007	1.0002	0.0008	1.0002	0.0008
THOR	1.0000	0.0006	1.0054	0.0006	1.0054	0.0006	0.9988	0.0006	0.9988	0.0006
PUSH2O	1.0000	0.0010	0.9961	0.0008	0.9961	0.0008	1.0002	0.0008	1.0002	0.0008
HISHPG	1.0000	0.0110	1.0106	0.0006	1.0106	0.0006	1.0118	0.0006	1.0118	0.0006
PNL2	1.0000	0.0065	1.0035	0.0009	1.0035	0.0009	1.0046	0.0009	1.0046	0.0009
PNL33	1.0024	0.0021	1.0044	0.0007	1.0044	0.0007	1.0074	0.0008	1.0074	0.0008
RMS diff			0.55%		0.55%		0.50%		0.50%	

black: diff < 1 sig
blue: 1 sig < diff < 2 sig
red: 2 sig < diff

A, B ENDF/B-VI + T16 + SAB2002, from August 2004
H, I ENDF/B-VII data + endf70sab, from May 8, 2008

The results shown in Table 4 provide evidence that:

- When MCNP5-1.40 and MCNP5-1.50 are compiled with the same compiler and compiler options on the same computer hardware, identical results are produced when the same nuclear data libraries are used for each code.

- Using the ENDF/B-VI nuclear data libraries, MCNP5-1.40 and MCNP5-1.50 give identical results for each of the 31 problems in the Criticality Validation Suite.

- Using the ENDF/B-VII nuclear data libraries, MCNP5-1.40 and MCNP5-1.50 give identical results for each of the 31 problems in the Criticality Validation Suite.

- The overall agreement between calculated results and benchmark experiment measurements is significantly improved for the new ENDF/B-VII data libraries, compared to the previous ENDF/B-VI+T16 libraries.

3. Results for Analytical Criticality Verification Suite

The analytical criticality verification suite [4] consists of 75 criticality problems for which exact results for k-effective are available from the literature. Reference [4] is included with the MCNP5-1.50 release documentation. A set of 10 problems was selected (Problems 11, 14, 18, 23, 32, 41, 44, 54, 63, 75) and run using both MCNP5-1.40 and MCNP5-1.50. These problems use a special set of cross-section data libraries, as specified in [4], and not the normal ENDF/B-VI or ENDF/B-VII data libraries distributed with MCNP5. Table 5 shows the results from these calculations, performed on a Mac Pro (2 quad-core Intel Xeon cpus, Mac OS X 10.4.11, Intel Fortran compiler 10).

For these problems, results calculated by MCNP5-1.40 and MCNP5-1.50 match each other exactly. Compared to the exact analytic benchmark results, 9 out of 10 cases for MCNP5-1.40 and MCNP5-1.50 agree with the exact results within one standard deviation, and 1 case (prob44) agrees with the exact result within 2 standard deviations.

Table 5. Analytical Criticality Verification Problems – Mac OS X

	Exact Results	MCNP5-1.40		MCNP5-1.50	
case	Keff	Keff	std-dev	Keff	std-dev
prob11	2.25000	2.25000	0.00000	2.25000	0.00000
prob14	1.00000	1.00006	0.00010	1.00006	0.00010
prob18	1.00000	1.00005	0.00011	1.00005	0.00011
prob23	1.00000	1.00000	0.00006	1.00000	0.00006
prob32	1.00000	0.99995	0.00011	0.99995	0.00011
prob41	1.00000	1.00003	0.00007	1.00003	0.00007
prob44	2.68377	2.68382	0.00003	2.68382	0.00003
prob54	1.00000	1.00007	0.00013	1.00007	0.00013
prob63	1.00000	0.99993	0.00006	0.99993	0.00006
prob75	1.60000	1.59999	0.00001	1.59999	0.00001

Table 6 shows results for this set of 10 problems when they were run with MCNP5-1.50 after the code was compiled with several compilers on Windows. The results using the different compilers match each other (and the Mac results) exactly for 9 out of 10 cases, and show only small roundoff differences for the case “prob44”. Similar to the Mac results, 9 out of 10 cases for all compilers match the exact results within 1 standard deviation, and 1 case matches the exact results within 2 standard deviations.

Table 6. Analytical Criticality Verification Problems - Windows

case	Keff-exact	Intel 10		Absoft 10		g95		portland	
		Keff	std-dev	Keff	std-dev	Keff	std-dev	Keff	std-dev
prob11	2.25000	2.25000	0.00000	2.25000	0.00000	2.25000	0.00000	2.25000	0.00000
prob14	1.00000	1.00006	0.00010	1.00006	0.00010	1.00006	0.00010	1.00006	0.00010
prob18	1.00000	1.00005	0.00011	1.00005	0.00011	1.00005	0.00011	1.00005	0.00011
prob23	1.00000	1.00000	0.00006	1.00000	0.00006	1.00000	0.00006	1.00000	0.00006
prob32	1.00000	0.99995	0.00011	0.99995	0.00011	0.99995	0.00011	0.99995	0.00011
prob41	1.00000	1.00003	0.00007	1.00003	0.00007	1.00003	0.00007	1.00003	0.00007
prob44	2.68377	2.68377	0.00003	2.68382	0.00003	2.68385	0.00003	2.68382	0.00003
prob54	1.00000	1.00007	0.00013	1.00007	0.00013	1.00007	0.00013	1.00007	0.00013
prob63	1.00000	0.99993	0.00006	0.99993	0.00006	0.99993	0.00006	0.99993	0.00006
prob75	1.60000	1.59999	0.00001	1.59999	0.00001	1.59999	0.00001	1.59999	0.00001

4. Results for the Shielding Validation Suite

The MCNP Radiation Shielding Validation Suite was used to assess how coding changes in the latest release of MCNP, MCNP5 Release 1.50, affect results in typical radiation shielding simulations. The MCNP Radiation Shielding Validation Suite consists of 19 benchmark problems documented in References [5-7]. The results of the test problems calculated with MCNP5-1.50 have been compared with results calculated with the previous release of MCNP5-1.40. The calculations for the comparison between MCNP5-1.40 and MCNP5-1.50 used nuclear data from ENDF/B-VI.

12 of the 19 benchmark problems run with MCNP5-1.50 resulted in identical output, *mctal*, and weight window output files compared to the corresponding files generated with MCNP5-1.40 (minor changes in output layout occurred with one of these 12 problems). 7 of the 12 benchmark problems run with MCNP5-1.50 did not produce the same results as the results obtained with MCNP5-1.40. These 7 problems resulted in a different particle history sequence as the baseline runs. The size of the differences, as output by the MCNP5 test system, between the baseline runs and the MCNP5-1.50 results are listed in Table 7. The CPU time execution times for each of the problems run with MCNP5-1.40 and MCNP5-1.50 are listed in Table 8.

Each of the 7 problems that did not track the baseline runs involved point detectors and photon transport. The differences in these 7 runs were traced to a new call to invoke photon Doppler broadening for next event estimators (F5 tallies), to a new method for handling how photons are banked during the simulation of positron-electron annihilation, and to removing the Hastings approximation from the Klein-Nishina formula evaluations for detectors. To ensure that these differences were only due to these two changes the old method of handling positron-electron annihilation was added to MCNP5-1.50 and these 7

Table 7. Test Summary for MCNP5/1.50 comparison to MCNP5 Release 1.40

```
MCNP     = /users/jsweezy/MCNP/dev/MCNP5_CVS/MCNP5/Source/src/mcnp5
CONFIG   = plot seq intel rossi
OS=Linux, TEMPLATES=Linux, NMPI=1, NTRD=1
XSTYPE   = 1
TEST_DIR = /users/jsweezy/MCNP/dev/MCNP5_CVS/MCNP5/Testing/VALIDATION_SHIELDING
```

CASE	OUTP diff	MCTAL diff	WWOUT diff	PTRAC diff	MESH tally diff
BE08	0	0	0	0	0
C29	0	0	0	0	0
CCR20	0	0	0	0	0
COAIR	5898	1140	0	0	0
COTEF	188672	2874	0	0	0
FE09	0	0	0	0	0
FS1ONN	0	0	0	0	0
FS3OFN	0	0	0	0	0
FS3ONP	708773	8186	9418	0	0
FS7OFP	760392	8186	9708	0	0
FS7ONN	0	0	0	0	0
H2O19	0	0	0	0	0
KERMIN	186118	5468	0	0	0
LI616	0	0	0	0	0
N31	0	0	0	0	0
PB14	0	0	0	0	0
SKYINP	258556	11142	0	0	0
SMAIR	200	0	0	0	0
SMTEF	248495	2874	0	0	0

```
>>> output        file diffs are in files:  difo??
>>> mctal         file diffs are in files:  difm??
>>> weight window file diffs are in files:  dife??
>>> ptrac         file diffs are in files:  difp??
>>> mesh tally    file diffs are in files:  dift??
---------------------------------------------------
```

tests were re-run with photon Doppler broadening disabled using the 5th entry on the PHYS:p card. The results of these 7 tests, run with photon Doppler broadening disabled using the modified version of MCNP5-1.50 and MCNP5-1.40, produced identical output, *mctal*, and weight window output files (except for some minor changes in the output layout)

These results were obtained on LANL's Flash cluster, which uses 64-bit Linux on 64-bit AMD Opteron Processors. Both MCNP5-1.50 and MCNP5-1.40 were compiled with Intel Fortran version 9.1.037, using the *–r8* option.

Table 8. CPU execution times for the MCNP Radiation Shielding Validation Suite problems.

Benchmark Problem	MCNP5/1.40 runtime (secs.)	MCNP5/1.50 runtime (secs.)	Increase in runtime from MCNP5/1.40 to MCNP5/1.50 (%)
BE08	31.71	33.86	6.8%
C29	41.61	43.32	4.1%
CCR20	67.05	69.04	3.0%
COAIR	9.74	10.66	9.4%
COTEF	467.48	506.87	8.4%
FE09	34.17	35.73	4.6%
FS1ONN	124.61	127.72	2.5%
FS3OFN	115.01	120.38	4.7%
FS3ONP	1185.26	1271.49	7.3%
FS7OFP	1508.26	1512.46	0.3%
FS7ONN	116.82	118.21	1.2%
H2O19	65.15	66.82	2.6%
KERMIN	100.21	105.55	5.3%
LI616	106.07	107.39	1.2%
N31	91.33	91.95	0.7%
PB14	73.62	74.86	1.7%
SKYINP	236.74	112.83	-52.3%
SMAIR	7.62	8.22	7.9%
SMTEF	1934.13	2080.13	7.5%
		Avg:	1.4%

5. Summary & Conclusions

The release notes for MCNP5-1.50 [12] describe the new features that are part of MCNP5-1.50 and a number of bugs in previous versions that have been fixed. Each of the coding changes for the new features and bug-fixes was independently checked to ensure that the changes were correct and did not interfere with the overall correctness of MCNP5 calculations.

The verification/validation testing described in the current report constitutes a set of integrated tests for a variety of criticality and shielding problems. The principal goal of this integrated testing is to ensure that the entire collection of changes in MCNP5 in going from MCNP5-1.40 to MCNP5-1.50 does not disrupt the integrity, correctness, and reliability of MCNP5 results for a varied set of typical application problems. In addition, we have provided some initial indication of the impact of moving from ENDF/B-VI data libraries to ENDF/B-VII data libraries.

The conclusions of the testing described in this report can be summarized by:

- When MCNP5-1.40 and MCNP5-1.50 are compiled and run on the same computer hardware, using the same compiler, compiler options, code physics options, and data libraries, then the two versions of MCNP5 produce identical results.

- The above statement is true, regardless of whether the code is run sequentially with 1-CPU, using threaded parallelism with multiple CPUs, using MPI parallelism with multiple CPUs, or using both threaded and MPI parallelism with multiple CPUs.

- When different compilers, compiler options, or computer hardware are used, MCNP5 results may differ slightly due to computer arithmetic roundoff. The observed differences were expected, reasonable, and explainable, with all results agreeing within statistics. The observed differences do not provide any indication of coding errors, execution errors, or data errors.

- In moving from ENDF/B-VI data libraries to ENDF/B-VII data libraries, no anomalies, surprises, or suspicious results were found. For the Criticality Validation Suite, using the ENDF/B-VII data libraries leads to significant improvement in the agreement with experimental benchmark measurements. (Further testing and validation of the ENDF/B-VII data libraries will be left to "experts" from the LANL X-1 Nuclear Data Team, the CSWEG participants, and others involved with verification/validation efforts.)

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