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Verification of MCNP5-1.60 and MCNP6.1 for Criticality Safety Applications

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INTRODUCTION

Several suites of verification/validation benchmark problems were run in early 2013 to verify that both MCNP5-1.60 [1,2] and MCNP6.1 [3] are performing correctly for criticality safety applications. Results from these benchmark suites were compared with results from previously verified versions of MCNP5 [4-6].

MCNP5-1.60 is the production version of MCNP5 included in RSICC releases in October 2010, July 2011, February 2012, and January 2013. MCNP6 is the merger of MCNP5 and MCNPX capabilities. MCNP6 includes all of the features for criticality safety calculations that are available in MCNP5-1.60, and many new features largely unrelated to nuclear criticality safety calculations. Beta versions of MCNP6 were distributed during 2012-2013 to allow advanced users to test the code in their fields of expertise. Release of the production version of MCNP6, called MCNP6.1, to RSICC is targeted for mid-2013. It includes MCNP6.1, MCNP5-1.60, MCNPX-2.70, the new ENDF/B-VII.1 data libraries, and an updated MCNP Reference Collection.

Several standard criticality benchmark suites [8-10] were used for the verification calculations:

- **VERIFICATION_KEFF** – A suite of criticality problems for which exact analytical results are available,
- **VALIDATION_CRITICALITY** – 31 *ICSBEP* [11] problems, using ENDF/B-VII.0,
- **VALIDATION_CRIT_EXPANDED** - 119 *ICSBEP* problems, using ENDF/B-VII.0 and ENDF/B-VII.1,
- **CRIT_LANL_SBCS** – 194 *ICSBEP* problems used by the LANL criticality safety group, using ENDF/B-VI.

METHODOLOGY AND BACKGROUND

For the **VALIDATION_CRIT_EXPANDED** Suite, all problems were also run with both ENDF/B-VII.0 [7] and ENDF/B-VII.1 [8] nuclear data libraries. The ENDF/B-VII.1 libraries were recently released and will be the default nuclear data for MCNP5 and MCNP6 in the upcoming RSICC production release of MCNP6.1.

An important part of the recent testing was a comparison of results obtained from MCNP5-1.60 and MCNP6.1 after they were recompiled using different versions of the Intel Fortran compiler. It should be noted that Fortran compilers are complex software programs, and all such programs have bugs. Testing MCNP using different versions of the Fortran compiler helps to verify that both MCNP and the Fortran compilers are performing correctly for criticality safety applications. It is also important to perform the MCNP and Fortran compiler testing on different computer operating systems, e.g., Windows, Linux, and Mac OS X, since codes and compilers sometimes perform differently on different systems.

In Reference [5], it was demonstrated that results from MCNP5 and MCNP6 compiled with different versions of the Intel Fortran compilers agree exactly for nearly all problems, and differ but agree within statistics for a few problems. While there will always be some roundoff differences due to the noncommutative and nonassociative nature of computer arithmetic, and the rearrangement of the order of operations by optimizing compilers, References [5-6] demonstrated that the roundoff differences are entirely acceptable, not errors, and recommended that all future MCNP development be carried out with the Intel 12 (current) Fortran compiler.

All of the testing performed recently was done in a parallel mode, using OpenMP threading with 8-16 cpu-cores. For all systems, we have used the "*-O1*" optimization level. Past testing typically showed only small gains in performance with higher optimization levels, at the expense of tremendous complications in verification due to small roundoff differences. We discourage users from invoking higher optimization levels, unless they are willing to also perform the necessary additional verification of code correctness.

In general, we try to choose options for different Fortran compilers and computer platforms that are as consistent as possible for building MCNP. Nevertheless, computer roundoff differences will occur with different compilers/hardware. Roundoff differences are not considered errors. Careful examination of these differences is necessary in the verification process to ensure that these differences are due solely to roundoff, and not to errors in coding or compilers.

Table I. MCNP6.1 Results for Analytic Keff Benchmarks

Case	Name	Analytic Exact keff	MCNP_Results keff	std
prob11	Ua-1-0-IN	2.25000	2.25000	0.00000
prob14	Ua-1-0-SP	1.00000	1.00006	0.00010
prob18	Uc-H2O(2)-1-0-SP	1.00000	1.00005	0.00011
prob23	UD2O-1-0-CY	1.00000	1.00000	0.00006
prob32	PUa-1-1-SL	1.00000	0.99995	0.00011
prob41	UD2Ob-1-1-SP	1.00000	1.00003	0.00007
prob44	PU-2-0-IN	2.68377	2.68377	0.00003
prob54	URRa-2-0-SL	1.00000	1.00007	0.00013
prob63	URRd-H2Ob(1)-2-0-ISLC	1.00000	0.99993	0.00006
prob75	URR-6-0-IN	1.60000	1.59999	0.00001

VERIFICATION_KEFF PROBLEMS - MCNP6

Table I shows the K_{eff} results for 10 benchmark problems from the **VERIFICATION_KEFF** suite run using MCNP6.1 compiled with the Intel-12 Fortran compiler. The problems were run on a Mac Pro computer using a 64-bit executable, 2 quad-core Xeon processors, OS X 10.6.8, and 8 threads. These analytic problems use 1-group cross-sections. The MCNP6.1 results are compared with the exact analytic results for K_{eff}. No significant differences are observed in Table I.

VALIDATION_CRITICALITY SUITE – MCNP5 VS MCNP6 USING ENDF/B-VII.0 NUCLEAR DATA

Table II shows the K_{eff} results for 31 benchmark problems for MCNP5-1.60 compiled with the Intel-10 and Intel-12 Fortran compilers, and MCNP6.1 compiled with the same Intel-12 compiler. The Intel-10 compiler generates only 32-bit executables; the Intel-12 compiler generates 64-bit executables. The problems were run on a Mac Pro computer using 2 quad-core Xeon processors, OS X 10.6.8, and 8 threads.

To simplify the comparisons, **Table II** shows the MCNP5-1.60 Intel-12 results and differences that arise for MCNP5-1.60 Intel-10. Cases that show differences are highlighted in green in both tables.

For the 4 MCNP5-1.60 cases that show differences between the Intel-10 and Intel-12 versions, the differences are within statistics and indicate computer roundoff (most likely from reordering of arithmetic due to compiler optimization), not errors in either MCNP or the Intel compilers. These differences are exactly the same as those seen in 2012 for the previous verification.

Using the Intel-12 compiler, results for MCNP5-1.60 and MCNP6.1 match exactly for all 31 cases. No differences in results were seen, when the same Intel Fortran compiler was used for each code. MCNP6.1 compiled with the Intel-12 compiler in 64-bit addressing mode is roughly 30% slower than MCNP5-1.60.

The **VALIDATION_CRITICALITY** Suite was also run with MCNP6.1 on a Windows computer system. MCNP6.1 was compiled using the Intel 12.1.5 Fortran compiler (with 64-bit addressing) on a system running Windows 7 Professional (Service Pack 1). All of the results for this suite of problems exactly matched the results obtained on Mac OS X and Linux systems.

VALIDATION_CRIT_EXPANDED SUITE – MAC, LINUX

MCNP5 & MCNP6 – Fortran Compiler Checks, Mac

This testing involved shortened versions of the 119 problems in the Expanded Criticality Validation Suite. The purpose was simply to look for any apparent differences in using the Intel-10 and Intel-12 Fortran compilers. Any absolute results should be discounted, since the problems were just run mechanically without regard to proper convergence.

Reference [6] shows the full set of K_{eff} results from MCNP5-1.60 using the Intel-10 and Intel-12 compilers, and the K_{eff} differences for MCNP6.1. One of the 119 cases showed minor roundoff differences between MCNP5-1.60 compiled with Intel-10 vs Intel-12. All of the Intel-12 MCNP5-1.60 and MCNP6.1 results agreed exactly in these shortened tests. The Intel-10 vs Intel-12 differences for MCNP5-1.60 are judged to be insignificant, and simply the normal roundoff differences between the two codes that are expected when running very many calculations.

MCNP5 & MCNP6 – ENDF/B-VII.0, Linux

Reference [6] shows the full set of K_{eff} results from MCNP5-1.60 and the K_{eff} differences for MCNP6.1 for the 119 problems in the Expanded Criticality Validation Suite (run in the standard way; not shortened). Both sets of calculations were run on a Linux cluster using 16 OpenMP threads and the same Intel-12 compiler with 64-bit executables. Four of the 119 cases showed minor roundoff differences between MCNP5 and MCNP6 results. Three of the cases showed roundoff differences less than 1σ, and the other case showed roundoff of just over 1σ. These differences are judged to be insignificant, and simply the normal roundoff differences between the

Table II. MCNP5 & MCNP6 VALIDATION_CRITICALITY Suite, with Different F90 Compilers – Diffs, Mac

```
mcnp5_10_70 = mcnp5-1.60, Intel 10, endf/b-vii.0
mcnp5_12_70 = mcnp5-1.60, Intel 12, endf/b-vii.0
mcnp6_12_70 = mcnp6.1,    Intel 12, endf/b-vii.0

Differences relative to reference:   mcnp5_12_70
  *'s indicate differences > 1, 2, or 3 std
```

	mcnp5_10_70		mcnp5_12_70		mcnp6_12_70	
	deltak	std	keff	std	deltak	std
U233 Benchmarks						
JEZ233	0.0000	(8)	0.9989	(5)	0.0000	(8)
FLAT23	0.0000	(9)	0.9990	(7)	0.0000	(9)
UMF5C2	0.0000	(8)	0.9931	(5)	0.0000	(8)
FLSTF1	0.0000	(15)	0.9830	(11)	0.0000	(15)
SB25	0.0000	(14)	1.0053	(10)	0.0000	(14)
ORNL11	0.0000	(5)	1.0018	(4)	0.0000	(5)
HEU Benchmarks						
GODIVA	0.0000	(8)	0.9995	(5)	0.0000	(8)
TT2C11	**0.0010**	**(10)**	1.0008	(7)	0.0000	(9)
FLAT25	0.0000	(9)	1.0034	(7)	0.0000	(9)
GODIVR	0.0000	(9)	0.9990	(7)	0.0000	(9)
UH3C6	0.0000	(11)	0.9950	(8)	0.0000	(11)
ZEUS2	**0.0002**	**(9)**	0.9972	(7)	0.0000	(9)
SB5RN3	0.0000	(18)	0.9985	(13)	0.0000	(18)
ORNL10	0.0000	(5)	0.9993	(4)	0.0000	(5)
IEU Benchmarks						
IMF03	0.0000	(8)	1.0029	(5)	0.0000	(8)
BIGTEN	0.0000	(7)	0.9945	(5)	0.0000	(7)
IMF04	0.0000	(8)	1.0067	(5)	0.0000	(8)
ZEBR8H	**-0.0001**	**(7)**	1.0196	(5)	0.0000	(7)
ICT2C3	0.0000	(9)	1.0037	(7)	0.0000	(9)
STACY36	0.0000	(8)	0.9994	(5)	0.0000	(8)
LEU Benchmarks						
BAWXI2	0.0000	(9)	1.0013	(7)	0.0000	(9)
LST2C2	0.0000	(8)	0.9940	(5)	0.0000	(8)
Pu Benchmarks						
JEZPU	0.0000	(8)	1.0002	(5)	0.0000	(8)
JEZ240	0.0000	(8)	1.0002	(5)	0.0000	(8)
PUBTNS	0.0000	(8)	0.9996	(5)	0.0000	(8)
FLATPU	0.0000	(9)	1.0005	(7)	0.0000	(9)
THOR	0.0000	(9)	0.9980	(7)	0.0000	(9)
PUSH2O	0.0000	(9)	1.0012	(7)	0.0000	(9)
HISHPG	**0.0004**	**(7)**	1.0118	(5)	0.0000	(8)
PNL2	0.0000	(12)	1.0046	(9)	0.0000	(12)
PNL33	0.0000	(9)	1.0065	(7)	0.0000	(9)

two codes that are expected when running very many calculations.

MCNP6 – ENDF/B-VII.0 AND ENDF/B-VII.1, LINUX

Reference [6] shows the full set of K_{eff} results for MCNP6.1 using ENDF/B-VII.0 and ENDF/B-VII.1 nuclear data for the 119 problems in the Expanded Criticality Validation Suite (run in the standard way; not shortened). Both sets of calculations were run on a Linux cluster using 16 OpenMP threads and the same Intel-12 compiler and a 64-bit executable.

Overall ENDF/B-VII.1 performs (on average) slightly better than ENDF/B-VII.0. The new dataset kept the ENDF/B-VII.0 evaluations for the major actinides, with the exception of the inelastic scattering cross section in ^{233}U and the delayed neutron decay constant data for all major actinides, and focused on minor actinides, structural materials, and light elements. Most importantly, there is no particular set of cases where ENDF/B-VII.1 performs worse than ENDF/B-VII.0, so most users should be able to switch data versions. References [7] and [8] provide extensive results from testing the ENDF/B-VII.1 nuclear data libraries on a wide range of problems.

SUMMARY AND CONCLUSIONS

Table III provides a summary of the verification results for the recent testing of MCNP5-1.60 and MCNP6.1 for criticality safety applications. The general conclusions from this testing are:

- Both MCNP5-1.60 and MCNP6.1 perform correctly for criticality safety applications.
- While small differences were noted for a few cases, these are strictly due to computer roundoff and are not a concern for verification/validation.
- MCNP5-1.60 and MCNP6.1 yield the same results on different computer platforms – Mac OS X, Linux, and Windows – for criticality safety applications.
- MCNP5-1.60 and MCNP6.1 yield the same results using OpenMP threading and/or MPI message-passing parallelism.
- Using the Intel-12 compiler and 64-bit addressing produces roughly a 20% speedup in the MCNP executables compared to using older compilers.
- MCNP6.1 runs roughly 30% slower than MCNP5-1.60. Causes for the MCNP6.1 performance reduction are under investigation.

As a result of this testing, it is recommended that all future development for MCNP be accomplished using the latest Fortran compiler, Intel-12, rather than older versions of the compiler. Using the Intel-12 Fortran compiler with 64-bit addressing permits the solution of very large problems that could not be run with older compilers and 32-bit addressing (where array sizes were limited to less than 2 GB), and also provides a speedup of roughly 30% in code execution.

Table III. Summary of Verification Results

VERIFICATION_KEFF – 10 analytical problems with exact K_{eff} results

- MCNP6.1, Intel-12 F90: **All results match**

VALIDATION_CRITICALITY – 31 ICSBEP Cases, ENDF/B-VII.0

- MCNP5-1.60 vs MCNP6.1
  - MCNP5 Intel-10 vs Intel-12: **4 diffs, within statistics**
  - MCNP5 & MCNP6, Intel-12: **All results match**

VALIDATION_CRIT_EXPANDED – 119 ICSBEP Cases, ENDF/B-VII.0

- MCNP5-1.60 vs MCNP6.1, SHORTENED PROBLEMS
  - MCNP5 Intel-10 vs Intel-12: **1 diff, within statistics**
  - MCNP5 & MCNP6, Intel-12: **All results match**
- MCNP5-1.60 vs MCNP6.1
  - MCNP5 & MCNP6, Intel-12: **4 diffs, within statistics**

Criticality safety analysts should consider testing MCNP6.1 on their particular problems and validation suites, to prepare for the migration from MCNP5 to MCNP6. It is expected that this migration should be accomplished within the next 1-3 years. Currently, no further development of MCNP5 is planned; all future MCNP improvements, bug fixes, and new capabilities are targeted only to MCNP6.

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