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## Verification of MCNP6.1, MCNP6.1.1, and MCNP6.2-pre for Criticality Safety Applications


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### INTRODUCTION

Several suites of verification/validation benchmark problems were run in early 2016 to verify that MCNP6.1 [1], MCNP6.1.1 [2], and MCNP6.2-pre are performing correctly for nuclear criticality safety applications (NCS). MCNP6.1 is the production version of MCNP® released in 2013; MCNP6.1.1 is the update released in 2014; MCNP6.2-pre is the pre-release development version of MCNP6.2, which is targeted for release in the near future. All versions of MCNP6 include all of the standard features for NCS calculations that have been available for the past 15 years, along with new features for sensitivity-uncertainty based methods for NCS validation [3]. Results from the benchmark suites were compared with results from previous verification testing [4-7].

Several standard criticality benchmark suites were used for the verification calculations:

- **VERIFICATION_KEFF** [8-10] – A suite of criticality problems for which exact analytical results are available,
- **VALIDATION_CRITICALITY** [11] – 31 *ICSBEP* [12] problems, using ENDF/B-VII.1 [13],
- **VALIDATION_CRIT_EXPANDED** [14] - 119 *ICSBEP* problems, using ENDF/B-VII.1.

### METHODOLOGY AND BACKGROUND

#### Analytic Criticality Suite

The VERIFICATION_KEFF verification suite has traditionally included 75 problems from [8-10] that were run as multigroup problems with MCNP. For the current testing, the verification suite has been completely revised and reconfigured [10,15].

It should be noted that previous usage of the VERIFICATION_KEFF suite made use of different coding in MCNP6, the multigroup coding, that is never used in realistic NCS calculations. With the modifications to the suite, the problems can now exercise the continuous-energy coding portions of MCNP6, the same coding that is used in realistic NCS calculations. (Of course, the continuous-energy physics in this suite is limited to 1-speed problems with elastic scattering, but at least the overall flow of the calculation stays involves the standard continuous-energy portions of MCNP6.)

#### Criticality Validation Suites

All of the testing for VALIDATION_CRITICALITY and VALIDATION_CRIT_EXPANDED was previously performed using ENDF/B-VII.0 nuclear data, so that comparisons could be made with the older MCNP5-1.60 code. (All versions of MCNP5 used the discrete $S(\alpha,\beta)$ thermal scattering model and data, and could not make use of the continuous-energy $S(\alpha,\beta)$ data released with ENDF/B-VII.1.) For the current testing, only the ENDF/B-VII.1 data was used, with continuous-energy $S(\alpha,\beta)$ thermal scattering.

Regarding bug fixes, MCNP6.1 had a small, infrequent error in dealing with the continuous-energy $S(\alpha,\beta)$ data: For some $S(\alpha,\beta)$ datasets at the very lowest energies (typically $10^{-5}$-$10^{-4}$ eV), NJOY lumps together scattering probabilities smaller than $10^{-6}$. MCNP6.1 did not handle that properly. This problem was fixed in MCNP6.1.1 (MCNP TeamForge Artifact 25705). While the effect of this problem has insignificant impact on results, there should be some very minor differences in a few results for problems with thermal scattering using MCNP6.1 and MCNP6.1.1. MCNP6.1.1 and MCNP6.2-pre use the same (corrected) coding for $S(\alpha,\beta)$ thermal scattering, so should give the same results.

#### Fortran Compiler Issues

An important part of the recent testing was a comparison of results obtained from MCNP6.1 and MCNP6.1.1 compiled with the Intel-12 Fortran compiler versus MCNP6.2-pre compiled with the Intel-15 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 NCS applications. However, when switching to a newer, different compiler, it is generally not possible to avoid some minor differences in results caused by different arithmetic roundoff between the compilers. 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. 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. Such roundoff differences are normally less than the statistical error of the results. In rare cases where that is not true, serious focused investigation into any differences must be performed and documented.

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. Performance testing 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.

## TESTING RESULTS

The criticality verification/validation suites were run on both Mac OS X and Linux systems with MCNP6.1, MCNP6.1.1, and MCNP6.2-pre. For Mac OS X, the suites were run on a Mac Pro computer using 64-bit executables, 12-core Xeon processor with 2 hyperthreads/core, OS X 10.9.5, and 14 MCNP threads. For Linux, the suites were run on a single node of a LANL cluster, with 64-bit executables, 8 dual-core Xeon processors, Chaos linux, and 16 MCNP threads. (While Windows test results are not presented in this work, regular testing is performed and results match other systems.)

## VERIFICATION_KEFF Suite

For the VERIFICATION_KEFF suite, MCNP results can be compared to exact results from analytic benchmark problems. For MCNP6.1 and MCNP6.1.1, results were reported in [4-6] for the analytic test problems run using the multigroup mode in MCNP6. In the current testing, MCNP6.2-pre was run using both multigroup and continuous-energy treatments for 38 analytic benchmark problems. The results from this testing are detailed in [10] and summarized here. The conclusions are:

- MCNP6.2-pre gives correct results for the analytic problems when run in multigroup mode. The absolute accuracy of the results is within 3 pcm ± 3 pcm. (1 pcm = 0.00001)
- MCNP6.2-pre gives correct results for the analytic problems when run in continuous-energy mode. The absolute accuracy of the results is within 3 pcm ± 3 pcm.

## VALIDATION_CRITICALITY Suite

**Table 1** shows the $K_{eff}$ results for 31 *ICSBEP* benchmark problems for MCNP6.1, MCNP6.1.1, and MCNP6.2-pre for both Mac OS X and Linux systems. To simplify the comparisons, the table shows the MCNP6.1 results and differences that arise for MCNP6.1.1 and MCNP6.2-pre. Cases that show differences are highlighted in green in the table.

To summarize the results of the present testing with the criticality validation suites and ENDF/B-VII.1 data, for 31 separate *ICSBEP* problems tested:

- On Mac OS X, 1 problem (ZEBR8H) out of 31 showed a difference between MCNP6.1.1 and MCNP6.2-pre. The difference was less than 2 combined standard deviations. For that problem, MCNP6.1 and MCNP6.1.1 agreed. On Linux, the same problem showed a difference from the Mac OS X results, but no differences among the Linux versions. The differences for this problem are most likely due to compiler roundoff differences.
- On both Mac OS X and Linux, 1 problem (ICT2C3) out of 31 showed a difference between MCNP6.1 and MCNP6.1.1. The difference was less than 2 combined standard deviations. For that problem, MCNP6.1.1 and MCNP6.2-pre agreed. This difference was almost certainly due to the S($\alpha$,$\beta$) bug fix, rather than roundoff differences.

## VALIDATION_CRIT_EXPANDED Suite

For this benchmark suite, 119 *ICSBEP* benchmark problems were run on both Mac OS X and Linux using MCNP6.1, MCNP6.1.1, and MCNP6.2-pre. No results are shown because: **For every one of the 119 benchmark problems, results matched exactly for all 6 different runs (i.e., 2 OS's, 3 code versions).**

## SUMMARY AND CONCLUSIONS

**Table 2** provides a summary of the verification results for the recent testing of MCNP6.1, MCNP6.1.1, and MCNP6.2-pre for NCS applications. The general conclusions from this testing are:

- MCNP6.1, MCNP6.1.1, and MCNP6.2-pre perform correctly for NCS applications.

**Table 1. Testing Results for VALIDATION_CRITICALITY Suite**

```
---------- MCNP Criticality V&V testing for NCSP ----------

        610_mac    = mcnp6.1       + Intel 12  + endf/b-vii.1 + macosx
        611_mac    = mcnp6.1.1b    + Intel 12  + endf/b-vii.1 + macosx
        620_mac    = mcnp6.2.0-pre + Intel 15  + endf/b-vii.1 + macosx
        610_lin    = mcnp6.1       + Intel 12  + endf/b-vii.1 + linux
        611_lin    = mcnp6.1.1b    + Intel 12  + endf/b-vii.1 + linux
        620_lin    = mcnp6.2.0-pre + Intel 15  + endf/b-vii.1 + linux

        Differences are relative to reference case:    610_12_71_mac
        *'s indicate differences > 1, 2, or 3 std
```

| | 610_mac keff std | 611_mac deltak std | 620_mac deltak std | 610_lin deltak std | 611_lin deltak std | 620_lin deltak std |
|---|---|---|---|---|---|---|
| U233 Benchmarks | | | | | | |
| JEZ233 | 1.0000 ( 5) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) |
| FLAT23 | 0.9974 ( 7) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) |
| UMF5C2 | 0.9960 ( 7) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) |
| FLSTF1 | 0.9845 (11) | 0.0000 (15) | 0.0000 (15) | 0.0000 (15) | 0.0000 (15) | 0.0000 (15) |
| SB25 | 0.9997 (10) | 0.0000 (14) | 0.0000 (14) | 0.0000 (14) | 0.0000 (14) | 0.0000 (14) |
| ORNL11 | 1.0018 ( 2) | 0.0000 ( 4) | 0.0000 ( 4) | 0.0000 ( 4) | 0.0000 ( 4) | 0.0000 ( 4) |
| HEU Benchmarks | | | | | | |
| GODIVA | 0.9988 ( 5) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) |
| TT2C11 | 1.0009 ( 8) | 0.0000 (11) | 0.0000 (11) | 0.0000 (11) | 0.0000 (11) | 0.0000 (11) |
| FLAT25 | 1.0034 ( 5) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) |
| GODIVR | 0.9989 ( 7) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) |
| UH3C6 | 0.9957 ( 8) | 0.0000 (11) | 0.0000 (11) | 0.0000 (11) | 0.0000 (11) | 0.0000 (11) |
| ZEUS2 | 0.9976 ( 7) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) |
| SB5RN3 | 0.9945 (13) | 0.0000 (18) | 0.0000 (18) | 0.0000 (18) | 0.0000 (18) | 0.0000 (18) |
| ORNL10 | 1.0001 ( 4) | 0.0000 ( 5) | 0.0000 ( 5) | 0.0000 ( 5) | 0.0000 ( 5) | 0.0000 ( 5) |
| IEU Benchmarks | | | | | | |
| IMF03 | 1.0019 ( 5) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) |
| BIGTEN | 0.9952 ( 5) | 0.0000 ( 7) | 0.0000 ( 7) | 0.0000 ( 7) | 0.0000 ( 7) | 0.0000 ( 7) |
| IMF04 | 1.0082 ( 5) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) |
| **ZEBR8H** | 1.0193 ( 5) | 0.0000 ( 8) | -0.0011 ( 8)* | -0.0011 ( 8)* | -0.0011 ( 8)* | -0.0011 ( 8)* |
| **ICT2C3** | 1.0023 ( 7) | 0.0012 ( 9)* | 0.0012 ( 9)* | 0.0000 ( 9) | 0.0012 ( 9)* | 0.0012 ( 9)* |
| STACY36 | 0.9981 ( 5) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) |
| LEU Benchmarks | | | | | | |
| BAWXI2 | 1.0025 ( 5) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) |
| LST2C2 | 0.9960 ( 5) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) |
| Pu Benchmarks | | | | | | |
| JEZPU | 0.9990 ( 5) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) |
| JEZ240 | 0.9999 ( 5) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) |
| PUBTNS | 0.9980 ( 7) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) |
| FLATPU | 1.0004 ( 7) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) |
| THOR | 0.9976 ( 5) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) |
| PUSH2O | 1.0013 ( 8) | 0.0000 (11) | 0.0000 (11) | 0.0000 (11) | 0.0000 (11) | 0.0000 (11) |
| HISHPG | 1.0121 ( 5) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) | 0.0000 ( 8) |
| PNL2 | 1.0050 (10) | 0.0000 (14) | 0.0000 (14) | 0.0000 (14) | 0.0000 (14) | 0.0000 (14) |
| PNL33 | 1.0068 ( 7) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) | 0.0000 ( 9) |
| Wall-clock: | 20.1 min | 12.6 min | 13.1 min | 18.8 min | 10.1 min | 10.4 min |
| Threads: | 14 | 14 | 14 | 16 | 16 | 16 |
| Rel. Speed: | 1.00 | 1.59 | 1.53 | 0.94 | 1.73 | 1.69 |

- The VERIFICATION_KEFF results indicate that all versions of MCNP6 are accurate to within 3±3 pcm when exact simple cross-sections are used for analytic benchmarks.
- While small differences were noted for 2 out of 150 *ICSBEP* problems, these are strictly due to computer roundoff or a minor bug-fix, and are not a concern for verification/validation.
- MCNP6.1, MCNP6.1.1, and MCNP6.2-pre yield the same results on different computer platforms – Mac OS X, Linux, and Windows – for NCS applications.

Criticality safety analysts should consider testing the latest version of MCNP6 on their particular problems and validation suites. No further development of MCNP5 is planned. All future MCNP improvements, bug fixes, user support, and new capabilities are targeted only to MCNP6.

**Table 2. Summary of Verification Results**

**VERIFICATION_KEFF** – 38 analytical 1-speed problems with exact $K_{eff}$ results

- MCNP6.2-pre: **Results are correct within 3±3 pcm**

**VALIDATION_CRITICALITY** – 31 ICSBEP Cases, ENDF/B-VII.1

- MCNP6.1, MCNP6.1.1, MCNP6.2-pre **1 roundoff diff, 1 bug-fix diff, 29 matches**

**VALIDATION_CRIT_EXPANDED** – 119 ICSBEP Cases, ENDF/B-VII.1

- MCNP6.1, MCNP6.1.1, MCNP6.2-pre **All results match on both Mac & Linux**

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