LA-UR-12-00179

Approved for public release;
distribution is unlimited.

Title:

MCNP6 Verification and Validation for the MCNPX_65 and MCNPX_EXTENDED Test Sets

Author(s):

Joe W. Durkee
Michael R. James

Intended for:

MCNP6 Release Documentation

MCNP6 Verification and Validation for the MCNPX_65 and MCNPX_EXTENDED Test Sets
January 11, 2012

Joe W. Durkee, Jr. , Michael R. James
Los Alamos National Laboratory
jdurkee@lanl.gov
505-665-0530
Fax: 505-665-2897
PO Box 1663, MS K575
Los Alamos, NM 87545

ABSTRACT

Verification and validation (v&v) testing of the MCNP6 code has been done using the test problems located in directories MCNPX_65 and MCNPX_EXTENDED in support of the MCNP/MCNPX code merger. This set consists of 561 tests and is designed to perform regression testing for MCNPX features. MCNP6 beta release version MCNP6_Beta2 (load date November 28, 2011 version 6.2.24) and MCNPX 2.7.0 have been executed and results compared for the test problems in the these directories.. Input changes in MCNP6 mean that some test problems contain execution options that required changes to the test problem to make the direct comparison of MCNP6 and MCNPX results. Many of the MCNP6 and v270 results compare well with each other. Results for a few test problems contain significant discrepancies. This v&v effort sought only to identify discrepancies, not to undertake corrections.

KEYWORDS: MCNP6, MCNPX; MCNPX_65, MCNPX_EXTENDED, verification and validation.

1. Introduction

Los Alamos National Laboratory (LANL) develops and maintains the MCNP (Brown, 2003a; Brown, 2003b) and, prior to the merger, the MCNPX™(Pelowitz, 2008) Monte Carlo N-Particle eXtended general-purpose radiation transport codes. A merged version of MCNP and MCNPX, MCNP6, will be released in 2012.

MCNP (MCNP6 and MCNPX) accommodates intricate three-dimensional geometrical models, continuous-energy transport of 36 different particle types plus heavy-ion transport, fuel burnup, and high-fidelity delayed-gamma emission. MCNP is written in Fortran 90, has been parallelized, and works on platforms including single-processor personal computers (PCs), Sun workstations, Linux clusters, and supercomputers. MCNP has thousands users throughout the world working on endeavors that include radiation therapy, reactor design, and homeland security.

Test problems from MCNPX were incorporated into MCNP6 as a part of the merger process. Predominantly, these were regression test problems that were designed to test one or more features. These test problems are located in test directories MCNPX_65 and MCNPX_EXTENDED in the Testing subdirectory of the MCNP6 file set. In order to gain confidence in the merger of MCNPX features into MCNP6, it was decided to test the answers produced from these problems in a side-by-side comparison of MCNPX 2.7.0 ("v270") and MCNP6. That v&v work is presented here.

2. MCNP6 verification and validation using MCNPX test models.

The v&v work was done as follows. MCNPX v270 was compiled with the Intel 10.0 compiler and the executable placed in the MCNP6/bin directory replacing the existing mcnp6 executable. This executable was then used to execute the test problems located in directories MCNPX_65 and MCNPX_EXTENDED. Each directory was run in turn by issuing the command 'make test EOL="" '[†]. It was also necessary to ensure that the files 'bertin' and 'phtlib' which are needed by MCNPX, were in the data path. The existing template files included with the MCNP6 distribution and generated by MCNP6 served as the baseline for the comparison.

The initial results checking was limited to mctal files. Contents of the mctal diff files produced by the "make" utility were viewed to assess differences. In many cases, the interpretation of the differences was trivial. Either no differences existed or differences were attributed to format differences in the MCNP6 and v270 mctal files. Some cases required that changes to inp files be made to enable proper v270 execution. In some cases, the eleventh entry to the lca card was removed , the phys:n eighth entry was moved to the 5th entry or the fmult card was replaced with settings on the phys:n 6th entry.

[†] This command suppresses the "dev-test eol" commands in the "make" file that are used for MCNP6 execution. These commands are contained in file …/MCNP6_Release/Testing/config/prundefine.mk.

In instances where more appreciable differences were noted, calculations were re-executed using more histories (SDEF) or cycles (kcode). Subjective judgment was applied to interpret results as being with or without appreciable difference.

No v&v work was done using other compilers, execution platforms, or MPI executables.

3. Verification and validation results.

The v&v computational results were compared by assessing differences in the mctal files. Differences in the outp files were looked at for cases where mctal file differences were significant. The tests are presented in the following subsections.

3.1. Test Set 1: MCNPX_65 models.

Good agreement was seen between mctal files for most problems. Discrepancies between MCNP6 and MCNPX v270 calculations were observed for the problems listed in Table 1. For models inp006 it was necessary to move phys:n 8^{th} entry. Also, changes in the way variance reduction games are handled show up in summary table comparisons, but the results from the two codes converge well. For inp113, NPS was increased 100x the default values and differences were still noted. The difference arises from the fact that this is a FLUKA test problem and MCNP6 uses LAQGSM for high-energy modeling. Model inp102 contains a “6” in the eleventh entry of the lca card, which v270 does not accommodate. Execution of inp102 by MCNP6 in “X mode” (using a “66” in the eleventh entry of the lca card) and v270 (with the eleventh entry absent) resulted in good agreement when NPS was increased to 10^4. Models inp115, inp116, inp309, and inp329 would not execute v270 due to the "tropt" option which is not treated by v270. Thus, no comparison of MCNP6 and v270 results was possible.

Table 1. Results for MCNPX_65 test models.

Test Model	Results for MCNP6 and v270
inp006	Ran to 100x, some small differences present
inp102	lca card. Ok for MCNP6 run in X mode NPS=10k
inp113	FLUKA test problem, not in MCNP6
inp115	Uses tropt-only MCNP6 has this option
inp116	Uses tropt-only MCNP6 has this option
inp309	Uses tropt-only MCNP6 has this option
inp329	Uses tropt-only MCNP6 has this option

3.2. Test Set 2: MCNPX_EXTENDED tests.

Calculations were executed for all subdirectories. No appreciable differences were found for test problems in subdirectories avr, class, classgeom, classvar, mbody, phys, push, test27a, test27b, testburn, testmcnp, and testmesh. Results in subdirectories for test problems with discrepancies are discussed next.

Initial execution of the heavyions test problems resulted in no differences with the exception of model inp80. This model contains "lca 10j 6". This prohibited the direct comparison of MCNP6 with v270 results because v270 does not treat this option. Makeshift tests were executed by 1) executing MCNP6 using the eleventh lca card entry set to 66, which caused MCNP6 execution in MCNPX mode, and 2) removing the eleventh lca card entry for v270 calculations. With this modification, calculations for all heavyions models resulted in no notable differences between MCNP6 and v270 as indicated in Table 2.1.

Table 2.1. Results for MCNPX_EXTENDED heavyions test models.

Test Model	Results for MCNP6 and v270
All	No appreciable differences

The test27d results revealed several differences as indicated in Table 2.2. Test models inp01, inp02, and inp03 initially failed to execute with a “form factor” error. These decks were modified by moving the “fcl:p=1” from the cell card for cell 1, which is fine for v270, to a separate card in the data section as “fcl:p 1 0 0”. Execution of MCNP6 was then successful.

Models inp12, inp13, and inp15 contain the FMULT card. Running the problems in MCNPX with the FMULT card removed and the equivalent setting used on phys:n card, resulted in no differences seen. Differences were noted in results for problem inp14 but this test uses a phys:n eighth entry in a way that is suspect and may be a mistake in the input file. MCNP6 and MCNPX interpret the eighth entry differently. In MCNPX is should be ignored, in MCNP6 it serves as the *tabl* transition energy.

Table 2.2. Results for MCNPX_EXTENDED test27d test models.

Test Model	Results for MCNP6 and v270
inp01	Form factor failure. Ok after move fcl:p=1 on cell to separate line for MCNP6
inp02	Form factor failure. Ok after move fcl:p=1 on cell to separate line for MCNP6
inp03	Form factor failure.

	Ok after move fcl:p=1 on cell to separate line for MCNP6
inp12	Remove FMULT card and used phys:n for MCNPX. No differences.
inp13	Remove FMULT card and used phys:n for MCNPX. No differences.
inp14	Phys:n 8th entry is present, suspect mistake in test problem.
inp15	Remove FMULT card and used phys:n for MCNPX. No differences.

The test27e results had many differences as listed in Table 2.3. Test models inp01, inp02, and inp03 include the LLNL fission multiplicity which requires changing input deck to invoke the LLNL Fission model from the phys:n card. Problem inp10 uses FT RES in combination with other tallies, which is a known bug, has not yet been fixed. Deck inp15 tests fission and activation by 20-MeV protons, inp16 fission by 22-MeV neutrons, and inp17 fission by 2000-MeV protons.

Table 2.3. Results for MCNPX_EXTENDED test27e test models.

Test Model	Results for MCNP6 and v270
inp01	Switch control from FMULT to phys:n, no differences
inp02	Switch control from FMULT to phys:n, no differences
inp03	Switch control from FMULT to phys:n, small differences?
inp10	Known bug, will be fixed in production release.
inp15	Some differences in delayed gamma treatment between MCNP6 and MCNPX
inp16	Some differences in delayed gamma treatment between MCNP6 and MCNPX
inp17	Differences seen

Initial testdndg results using the default settings in the test files produced some differences. Results for models inp01, inp02, inp03, and inp23 had large uncertainties. Execution using 10^5 histories suggested that the MCNP6 and v270 results were in sufficient agreement.

Test models inp41 and inp42 initially failed to execute v270 due to a data value ("6") in the eleventh place of the lca card. Consequently, direct comparison of MCNP6 with v270 results was not possible. Further testing was done by 1) executing MCNP6 using the eleventh lca card entry set to 66, which caused MCNP6 execution in MCNPX mode, and 2) removing the eleventh lca card entry for v270 calculations.

All test problems were in close agreement for MCNP6 and v270 as indicated in Table 2.4. The companion reports (Durkee, 2011a; Durkee, 2011b; Durkee, 2011c) contain extensive descriptions of delayed-particle v&v.

Table 2.4. Results for MCNPX_EXTENDED testdndg test models.

Test Model	Results for MCNP6 and v270
inp01	Base NPS poor. NPS 10^5 ok.
inp02	Base NPS poor. NPS 10^5 ok.
inp03	Base NPS poor. NPS 10^5 ok.
inp41	lca card. Ok for MCNP6 run in X mode.
inp42	lca card. Ok for MCNP6 run in X mode.

Calculations for all testincl models produced the following findings. Models inp103, inp108, inp22, inp25, inp28, inp86, and inp96 would not execute v270 due to a data value ("6") in the eleventh place of the lca card. Consequently, direct comparison of MCNP6 with v270 results was not possible. Further testing was done by 1) executing MCNP6 using the eleventh lca card entry set to 66, which caused MCNP6 execution in MCNPX mode, and 2) removing the eleventh lca card entry for v270 calculations.

Models 86 and 96 had discrepancies for the default 10^4 histories. When running 10^6 histories, MCNP6 failed with an error from CEM.

```
warning. CEM residual nuclei error, target za=  82208.
 nps =        67343      za = 1001     erg = 1.2000E+03
 Expire parameter is CEM residual nuclei error

 bad trouble in subroutine STOREP of mcrun

 source particle no.        67343

 starting random number =      113347954011057

 CEM residual nuclei error
      run terminated because of bad trouble.
```

This error has been noted and will be fixed in the production release.

Results for the testincl models are listed in Table 2.5.

Table 2.5. Results for MCNPX_EXTENDED testincl test models.

Test Model	Results for MCNP6 and v270
inp103	Differences for ref & 100x NPS
inp108	lca card. Ok for MCNP6 run in X mode.
inp114	Differences for ref & 100x NPS
inp22	lca card. Ok for MCNP6 run in X mode.
inp25	lca card. Ok for MCNP6 run in X mode.
inp28	lca card. Ok for MCNP6 run in X mode.
inp86	lca card. Discrepancies for MCNP6 run in X mode using default NPS = 10^4. For NPS = 10^6: MCNP6 fatal: CEM residual nuclide error MCNPX: executed to completion Bug will be fixed in production release.
inp96	lca card. Discrepancies for MCNP6 run in X mode using default NPS = 10^4. For NPS = 10^6: MCNP6 fatal: CEM residual nuclide error MCNPX: executed to completion Bug will be fixed in production release.

Calculations for all testmix models resulted in no appreciable differences between MCNP6 and v270 as indicated in Table 2.6. Execution of v270 using inp03 results in failure due to the presence of an lca card with eleven entries. Eliminating the eleventh entry enables v270 to execute with results that are not notably different from MCNP6.

Table 2.6. Results for MCNPX_EXTENDED testmix models.

Test Model	Results for MCNP6 and v270
All	No appreciable differences

Calculations for testpht between MCNP6 and v270 resulted in differences for many models as indicated in Table 2.7. This is expected because MCNP6 and v270 use different implementations of Pulse-Height Tally Variance Reduction.

Table 2.7. Results for MCNPX_EXTENDED testpht test models.

Test Model	Results for MCNP6 and v270
inp04e	Differences
inp04w	Differences
inp05e	Differences
inp05w	Differences
inp14e	Differences
inp14w	Differences
inp15e	Differences
inp15w	Differences
inp24w	Differences
inp25e	Differences
inp25w	Differences
inp31w	Differences

Calculations for testxnew models resulted in no appreciable differences for most test files. However, execution of inp12 using MCNP6 failed:

```
cycle    k(col)       ctm   entropy    active     k(col)    std dev
fom
     1   1.41516      0.00  3.95E+00
 Expire parameter is the energy of a source particle is zero or less.

 bad trouble in subroutine startp of mcrun

 source particle no.          583

 starting random number =       58958014849681

 the energy of a source particle is zero or less.
      run terminated because of bad trouble.
```

This issue relates to using the LLNL Fission model with KCODE. This combination is unsupported in MCNP6.

Table 2.8. Results for MCNPX_EXTENDED testxnew test models.

Test Model	Results for MCNP6 and v270
inp12	MCNP6 fails with source particle energy zero or less, LLNL Fission and KCODE unsupported.

Calculations for all testxold models resulted in no notable differences between MCNP6 and v270 as noted in Table 2.9.

Table 2.9. Results for MCNPX_EXTENDED testxold test models.

Test Model	Results for MCNP6 and v270
All	No appreciable differences

Calculations for all zrecoil models resulted in appreciable differences as shown in Table 2.10. Most of these changes were from the different input methods for fission multiplicity. This is expected because MCNP6 and v270 run differently.

Table 2.10. Results for MCNPX_EXTENDED zrecoil test models.

Test Model	Results for MCNP6 and v270
inp04	FMULT control shifted to phys:n, Ok for MCNP6 run in X mode.
inp06	FMULT control shifted to phys:n, Ok for MCNP6 run in X mode.
inp07	FMULT control shifted to phys:n, Ok for MCNP6 run in X mode.
inp55	FMULT control shifted to phys:n, Ok for MCNP6 run in X mode.
inp16	FMULT control shifted to phys:n, Ok for MCNP6 run in X mode.
inp17	FMULT control shifted to phys:n, Ok for MCNP6 run in X mode.
inp18	FMULT control shifted to phys:n, Ok for MCNP6 run in X mode.
inp19	FMULT control shifted to phys:n, Ok for MCNP6 run in X mode.
inp22	FMULT control shifted to phys:n, Ok for MCNP6 run in X mode.
inp23	FMULT control shifted to phys:n, Ok for MCNP6 run in X mode.
inp64	Uses antiparticle promotion, not in MCNPX

4. Summary and conclusions

In support of the MCNP/MCNPX code merger, a v&v study has been conducted to identify appreciable discrepancies between MCNP6 and MCNPX v2.7.0 results using MCNPX test problems located on directories MCNPX_65 and MCNPX_EXTENDED. This effort did always not extend to the identification of the underlying causes of the discrepancies. Differences have been noted for future attention.

MCNP6 beta release version MCNP6_Release (load date November 28, 2011 version 6.2.24) and MCNPX 2.7.0 were the code versions used. Comnparison of the test problems was done using executables for both codes to facilitate intercomparison of calculated results.

The initial screening of significant discrepancies was done using mctal files. In some instances, no differences in mctal files created by MCNP6 and v270 were noted. In others, trivial differences were noted regarding simple format changes in MCNP6 and v270 files.

For some results, differences were noted for the default number of histories or kcode settings. For such cases, the execution was redone using more histories, often 100 times more, or refined kcode parameters. This refinement sometimes resulted in reductions in the differences between MCNP6 and v270 to permit the qualitative assessment of agreement. Other times, differences remained.

Some input files contained a "6" in the eleventh location of the lca card. v270 does not accommodate this entry. Consequently, a direct comparison of MCNP6 and v270 was not possible. Comparison of MCNP6 execution in "X mode" was done by changing the "6" to a "66" for MCNP6. Companion v270 execution was done by omitting the entry in the eleventh column of the lca card. In many instances, execution of MCNP6 in "X mode" resulted in insignificant differences. In other instances, differences remained.

Some test models contain the "tropt" option. This option is treated by MCNP6 but is not treated by MCNPX. Comparison of results for such models was not possible.

Since these test sets were primarily used for regression testing, it was not practical to identify which results were significant in each case. The methodology was also subjective for identifying "significant" differences in test answers. Overall, there are a number of test problems on test directories MCNPX_65 and MCNPX_EXTENDED for which appreciable discrepancies exist between MCNP6 and v270 results. However, for the majority of test problems, the codes run equivalently and give the same answers.
The v&v test results here are a companion to results summarized in the document, "MCNP6 Delayed-Particle Verification and Validation, which is in preparation.

References

Brown F.B., ed., April 2003a. "MCNP–A General Monte Carlo N–Particle Transport Code, Version 5, Volume I: Overview and Theory," Los Alamos National Laboratory report LA-UR-03-1987, Ch 2 pp. 182–185.

Brown F.B., ed., April 2003b. "MCNP–A General Monte Carlo N–Particle Transport Code, Version 5, Volume II: User's Guide," Los Alamos National Laboratory report LA-CP-03-0245, Ch 3 pp. 31–32.

Durkee Joe W., Jr., February 2011. "MCNP6 Delayed-Particle Verification and Validation," Los Alamos National Laboratory report LA-UR-11-01375.

Durkee Joe W., Jr., June 2011. "MCNPX Delayed-Particle Verification and Validation," Los Alamos National Laboratory report LA-UR-11-03315.

Pelowitz D.B., ed., April 2008. "MCNPX User's Manual Version 2.6.0," Los Alamos National Laboratory report LA-CP-07-1473.