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MCNP5-1.60 Release & Verification

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INTRODUCTION

The latest release of the MCNP5 [1] Monte Carlo code is designated MCNP5-1.60. It includes enhancements to several MCNP capabilities: maximum number of cells, surfaces, materials, and tallies; isotopic reaction rates for mesh tallies; and adjoint-weighting for computing effective lifetimes and delayed neutron parameters. In addition, there are many minor code modifications to fix reported bugs, output formats, error checking, and other difficulties present with previous versions of MCNP. In nearly all cases, the bug fixes addressed problems with infrequently-used combinations of code options. In some cases, the problems that are fixed date back to the 1990s, but were only recently reported and fixed. All previously existing code capabilities are preserved, including physics options, geometry, tallying, plotting, cross-section handling, etc. No errors were found that would affect the code results for basic criticality calculations.

Extensive verification and validation testing was performed, involving roughly 5,000 hrs of computing time. Tally results from MCNP5-1.60 are expected to match the tally results of problems that can be run with the previous MCNP5-1.51 [2,3], except where bugs were discovered and fixed. The bug fixes and enhancements are discussed in [4], supplemental pages for the MCNP manual are provided in [5], and verification/validation work is described in [6]. In the sections below, we summarize the code enhancements and provide some results from the verification/validation effort.

NEW FEATURES IN MCNP5-1.60

Adjoint-weighted Tallies for Point Kinetics Parameters

Many quantities in reactor physics involve adjoint or importance weighting. The adjoint response function used by MCNP5 for criticality calculations is the iterated fission probability. Lumped average parameters describing the kinetics for a reactor system can be derived from the linear Boltzmann equation, with the resulting parameters involving ratios of adjoint-weighted reaction rates. In particular, the neutron generation time Λ and the effective delayed neutron fraction β_{eff} are expressed as ratios of adjoint-weighted integrals. For the first time, MCNP5-1.60 includes the capability to generate adjoint-weighted reactor kinetics parameters from continuous-energy Monte Carlo. The theory, MCNP5 input instructions, and verification suite associated with this feature are described in [7,8].

Mesh Tallies for Isotopic Reaction Rates

MCNP5 has always had the capability to perform mesh tallies for fluxes and material reaction rates on an arbitrary, user-specified mesh that is independent of the actual problem geometry [1]. An important previous enhancement permitted users to specify a “wildcard” material number of *0* on the associated FM card, which caused the mesh tally routines to use the actual material number densities in the problem, which were dependent on a particle’s actual location in the problem geometry. This important capability to “wildcard” the number densities was previously limited to materials, and could not be used to obtain individual isotopic reaction rates. With MCNP5-1.60, use of the FM cards for mesh tallies has been extended to handle isotopic mesh tallies as well, so that users do not need to enter number densities directly for isotopic mesh tallies; the mesh tally routines can now find the actual problem materials and use the appropriate number densities in performing the isotopic reaction rate tallies. This enhancement to the mesh tally capabilities is described in detail in [6], along with input instructions and examples.

Increased Limits for Geometry, Tally, and Source Specifications

MCNP5-1.60 includes modifications that extend the limits on the number of cells, surfaces, materials, etc., from a maximum of 99,999 to 99,999,999. The maximum number of tally card identifiers is also raised from 999 to 9,999. Detailed discussion of these changes is found in [5]. The limit on the size of logical arrays for complicated cells is raised from 1,000 to 9,999. That is, a cell card specification may now include a list of up to 9,999 surfaces (with ± to denote sense), union operators (:), and parentheses.

Other Enhancements

The documentation for MCNP5-1.60 is organized in an easy to access, web-based format that can be viewed in any web browser. The documentation includes over 280 MB of reference material.

The *merge_mctal* and *merge_meshtal* utilities are used to merge separate *mctal* or *meshtal* files, respectively, from different independent MCNP5 jobs. Both were updated and made more general.

There are general enhancements to the build system, parallel processing efficiency, continue runs, random number generator options, number of nesting levels for universes, etc.

VERIFICATION AND VALIDATION TESTING

To verify that the MCNP5-1.60 is performing correctly, several suites of verification/validation problems were run. Results have been compared with previously verified versions of MCNP5, with experimental or analytic results, and with results from running on different computer hardware/software platforms. In addition, two new verification/validation suites have been added, the Kobayashi benchmarks with problems containing voids and ducts, and a set of benchmarks for reactor kinetics parameters. The testing suites are:

Regression - The standard MCNP5 Regression Test Suite [1,3] is expanded from 52 to 66 problems, with new tests added to cover new code features or to explicitly test that particular bugs are fixed. Previous analysis of MCNP5 indicated that the tests cover approximately 80-90% of the total lines of coding. The regression tests do not verify code correctness; they are used only for the purpose of detecting unintended changes to the code and for installation testing.

VALIDATION_CRITICALITY - The Criticality Validation Suite [9] consisting of 31 problems from the *International Handbook of Evaluated Criticality Benchmark Experiments* [10]. 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 in configurations that produce fast, intermediate, and thermal spectra. For each fuel type, there are cases with a variety of moderators, reflectors, spectra, and geometries. The cases in the suite were chosen to include a variety of configurations. The suite was modified to permit running with either ENDF/B-VI data libraries or the newer ENDF/B-VII.0 data libraries.

VERIFICATION_KEFF - Reference [11] 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 MCNP5-1.60 verification, ten of these analytic benchmark problems were run to high precision.

VALIDATION_SHIELDING - The Radiation Shielding Validation Suite [9,12] 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. This suite was overhauled to compare plots of results against experimental data.

KOBAYASHI - The “Kobayashi Benchmarks” [13] are added. This set of 3D benchmark problems consist of simple geometries that contain at least one void region and one mono-energetic, isotropic, cubic source region. Each configuration is simulated first with a purely absorbing and then with a fifty-percent scattering medium. Fluxes are calculated at various points throughout the geometries using point detector tallies. For the purely absorbing cases, there are exact solutions obtained using numerical integration. For the cases with scattering, reference solutions were computed by very long runs using the MVP Monte Carlo code [13]. Overall, for two cases of each of the three problems, 136 different fluxes were compared between computed MCNP5 results and the reference.

POINT_KINETICS - The Point Kinetics Validation suite [7,8]. MCNP5-1.60 has, for the first time, the ability to compute adjoint-weighted tallies in criticality calculations using only the existing random walks. References [7,8] detail the ability to compute reactor kinetics parameters: neutron generation times, Rossi-α, total and precursor-specific effective delayed neutron fractions, and average precursor decay constants. A series of verification and validation problems was added to the MCNP5 distribution. The verification problems are compared against both analytic solutions and with discrete ordinates results obtained from Partisn [14]. For validation, MCNP computes six values of Rossi-alpha and these values are compared against experimentally measured values experiments from the OECD/NEA benchmark handbook [10].

Verification calculations for MCNP5-1.60 were run on Mac OS X, Linux, and Windows computing systems. Extensive testing was performed using sequential execution (i.e., 1 CPU), threaded calculations using OpenMP with various numbers of threads, parallel message-passing using OpenMPI with various numbers of CPUs, and mixed threaded+MPI calculations using different combinations of threading and MPI. On each computer platform, several different Fortran-90 compilers were used in the testing. The total computing time used during the course of the testing was approximately 5,000 CPU-hours, over a span of several months calendar time. Results from these calculations have been compared to results from the previous, verified version of MCNP5 (Version 1.51), to known analytical results, and to results from experiments.

Representative results from the verification testing are shown in Tables I-III and Figure 1. Table I shows a comparison of reference results from MVP vs. results computed using MCNP5-1.60 for 1 of the 6 Kobayashi benchmark cases. Table II provides results from the Criticality Validation Suite using ENDF/B-VII.0 cross-section data, comparing experiment, the previous MCNP5-1.51, and MCNP5-1.60. Results from the new and previous versions of MCNP5 match exactly for Mac OS X; for Linux and Windows, typically 3-4 results show small roundoff differences (depending on compiler) and the other results match exactly between versions. Table III shows results from the kinetics parameter validation suite, including comparisons to experiment, exact analytic results, and Partisn S_n results. Figure 1 shows results from three of the eight pulsed sphere problems that were run, comparing experiment vs. MCNP5-1.60 results. Similar agreement is seen in the other pulsed sphere problems, the fusion shielding problems, and the skyshine benchmark.

CONCLUSIONS

Based on 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, MCNP5-1.60. We do not presume to declare MCNP5-1.60 as validated for any particular end-user application (that is the prerogative 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 MCNP5-1.60 verification testing. MCNP5-1.60 can be obtained from RSICC (*rsicc.ornl.gov).*

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Table I. Kobayashi Benchmark Results for Linux – Problem 1, Absorption + Scattering, 100M Histories

	x, y, z	Reference & Rel.Err.		MCNP-result & Rel.Err.		C/E
Detector Set A						
f1405	5, 5, 5	8.29e+0	0.0002	8.22e+0	0.0002	0.99
f1415	5,15, 5	1.87e+0	0.0001	1.86e+0	0.0002	1.00
f1425	5,25, 5	7.13e-1	0.0000	7.13e-1	0.0001	1.00
f1435	5,35, 5	3.84e-1	0.0000	3.84e-1	0.0001	1.00
f1445	5,45, 5	2.53e-1	0.0001	2.54e-1	0.0001	1.00
f1455	5,55, 5	1.37e-1	0.0007	1.37e-1	0.0005	1.00
f1465	5,65, 5	4.65e-2	0.0012	4.68e-2	0.0007	1.01
f1475	5,75, 5	1.58e-2	0.0020	1.59e-2	0.0008	1.00
f1485	5,85, 5	5.47e-3	0.0034	5.48e-3	0.0012	1.00
f1495	5,95, 5	1.85e-3	0.0062	1.83e-3	0.0019	0.99
Detector Set B						
f1505	5, 5, 5	8.29e+0	0.0002	8.22e+0	0.0002	0.99
f1515	15,15,15	6.63e-1	0.0000	6.63e-1	0.0001	1.00
f1525	25,25,25	2.68e-1	0.0000	2.69e-1	0.0001	1.00
f1535	35,35,35	1.56e-1	0.0001	1.57e-1	0.0001	1.00
f1545	45,45,45	1.04e-1	0.0001	1.04e-1	0.0002	1.00
f1555	55,55,55	3.02e-2	0.0006	3.01e-2	0.0009	1.00
f1565	65,65,65	4.06e-3	0.0007	4.08e-3	0.0015	1.01
f1575	75,75,75	5.86e-4	0.0012	5.89e-4	0.0034	1.01
f1585	85,85,85	8.66e-5	0.0020	8.73e-5	0.0087	1.01
f1595	95,95,95	1.12e-5	0.0038	1.16e-5	0.0236	1.03
Detector Set C						
f1605	5,55, 5	1.37e-1	0.0007	1.37e-1	0.0005	1.00
f1615	15,55, 5	1.27e-1	0.0008	1.28e-1	0.0005	1.00
f1625	25,55, 5	1.13e-1	0.0008	1.13e-1	0.0005	1.00
f1635	35,55, 5	9.59e-2	0.0009	9.65e-2	0.0006	1.01
f1645	45,55, 5	7.82e-2	0.0009	7.88e-2	0.0006	1.01
f1655	55,55, 5	5.67e-2	0.0011	5.65e-2	0.0007	1.00
f1665	65,55, 5	1.88e-2	0.0019	1.89e-2	0.0009	1.01
f1675	75,55, 5	6.46e-3	0.0031	6.50e-3	0.0012	1.01
f1685	85,55, 5	2.28e-3	0.0053	2.29e-3	0.0018	1.01
f1695	95,55, 5	7.93e-4	0.0089	8.00e-4	0.0029	1.01

Figure 1. Pulsed Sphere Problems

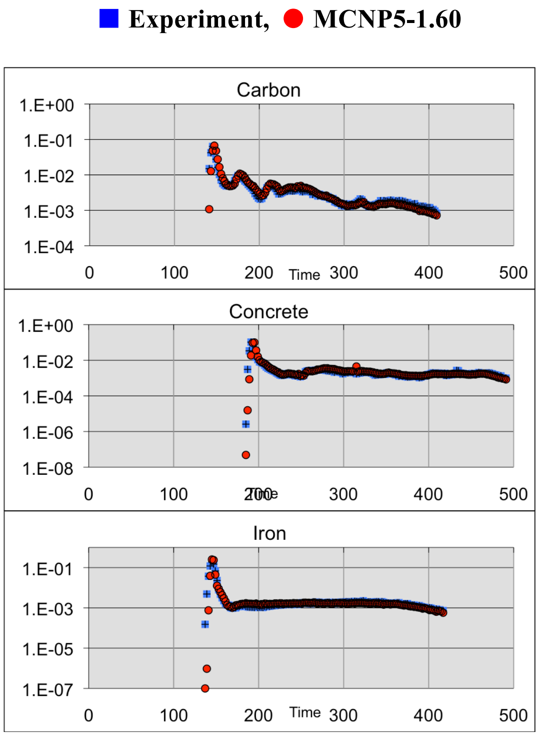

Table II. MCNP Criticality Validation Suite, Results on Mac OS X for ENDF/B-VII.0

	Experiment	MCNP5-1.51	MCNP5-1.60
U233 Benchmarks			
JEZ233	1.0000 (10)	0.9989 (6)	0.9989 (6)
FLAT23	1.0000 (14)	0.9990 (7)	0.9990 (7)
UMF5C2	1.0000 (30)	0.9931 (6)	0.9931 (6)
FLSTF1	1.0000 (83)	0.9830 (11)	0.9830 (11)
SB25	1.0000 (24)	1.0053 (10)	1.0053 (10)
ORNL11	1.0006 (29)	1.0018 (4)	1.0018 (4)
HEU Benchmarks			
GODIVA	1.0000 (10)	0.9995 (6)	0.9995 (6)
TT2C11	1.0000 (38)	1.0018 (8)	1.0018 (8)
FLAT25	1.0000 (30)	1.0034 (7)	1.0034 (7)
GODIVR	0.9985 (11)	0.9990 (7)	0.9990 (7)
UH3C6	1.0000 (47)	0.9950 (8)	0.9950 (8)
ZEUS2	0.9997 (8)	0.9974 (7)	0.9974 (7)
SB5RN3	1.0015 (28)	0.9985 (13)	0.9985 (13)
ORNL10	1.0015 (26)	0.9993 (4)	0.9993 (4)
IEU Benchmarks			
IMF03	1.0000 (17)	1.0029 (6)	1.0029 (6)
BIGTEN	0.9948 (13)	0.9945 (5)	0.9945 (5)
IMF04	1.0000 (30)	1.0067 (6)	1.0067 (6)
ZEBR8H	1.0300 (25)	1.0195 (6)	1.0195 (6)
ICT2C3	1.0017 (44)	1.0037 (7)	1.0037 (7)
STACY36	0.9988 (13)	0.9994 (6)	0.9994 (6)
LEU Benchmarks			
BAWXI2	1.0007 (12)	1.0013 (7)	1.0013 (7)
LST2C2	1.0024 (37)	0.9940 (6)	0.9940 (6)
Pu Benchmarks			
JEZPU	1.0000 (20)	1.0002 (6)	1.0002 (6)
JEZ240	1.0000 (20)	1.0002 (6)	1.0002 (6)
PUBTNS	1.0000 (30)	0.9996 (6)	0.9996 (6)
FLATPU	1.0000 (30)	1.0005 (7)	1.0005 (7)
THOR	1.0000 (6)	0.9980 (7)	0.9980 (7)
PUSH2O	1.0000 (10)	1.0012 (7)	1.0012 (7)
HISHPG	1.0000 (110)	1.0122 (5)	1.0122 (5)
PNL2	1.0000 (65)	1.0046 (9)	1.0046 (9)
PNL33	1.0024 (21)	1.0065 (7)	1.0065 (7)

Table III. MCNP Kinetics Parameter Validation Suite Results on Linux

	Benchmark_Results		MCNP_Results & Rel Err	
Comparison with Experiments Rossi-Alpha (1/ns or 1/us)				
GODIVA	-0.0011	2e-05	-0.001131	7e-6
JEZPU	-0.00064	1e-05	-0.000649	8e-6
BIGTEN	-0.000117	1e-06	-0.0001156	7e-7
FLAT23	-0.000267	5e-06	-0.0002931	3e-6
STACY29	-0.000122	4e-06	-0.0001222	9e-7
WINCO5	-0.001109	3e-06	-0.001124	1e-5
Comparison with Exact Analytic Solutions Generation Time (ns or us)				
ONEINF	10		9.999	0.00085
TWOINF	14.17		14.16	0.00275
Comparison with PARTISN Solutions Generation Time (ns or us)				
BARESLAB	9.793		9.792	0.00594
REFLSLAB	135.2		135.1	0.1068
THRESLAB	49.17		49.28	0.1018
INTRSLAB	112.1		112.7	0.4397
BARESPHR	1.721		1.722	0.00102
REFLSPHR	10.19		10.19	0.00737
SUBCSLAB	10.17		10.17	0.0073
SUPCSLAB	9.673		9.674	0.00526