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Advances in the Development and Verification of MCNP5 and MCNP6

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ABSTRACT

The MCNP Monte Carlo code has been used for high-fidelity analyses of criticality safety problems since the 1970s. This paper reviews recent advances in the development and verification of MCNP, including the current production release of MCNP5 and the beta release of MCNP6. End-users in all application areas need to be aware of the forthcoming MCNP6 release and begin planning for the transition to the new code in 2012 and beyond.

Key Words: MCNP, Monte Carlo, criticality safety

1 INTRODUCTION

The MCNP Monte Carlo code has been used for high-fidelity analyses of criticality safety problems since the 1970s. This paper reviews recent advances in the development and verification of MCNP, including the current production release of MCNP5 and the beta release of MCNP6.

The latest production release of MCNP5 is designated MCNP5-1.60 [1,2,3,4]. It includes enhancements to several MCNP capabilities and many minor code modifications to fix difficulties reported with previous versions of MCNP. Extensive verification and validation testing of MCNP5-1.60 was performed with a variety of compilers and computer platforms. No errors were found that would affect the code results for basic criticality calculations.

The MCNP6 Monte Carlo code has been under development since 2004, when a version of MCNP5 was modified to include capabilities for modeling high-energy protons. MCNP6 was used locally for the analysis of experiments involving proton radiography. Over the past 3 years, many additional capabilities for high-energy physics, depletion, and detector modeling have been merged from the MCNPX [5] Monte Carlo code into MCNP6. MCNP6 can currently model 36 different particle types as well as heavy ions. MCNP6 includes all features and capabilities found in MCNP5 and MCNPX, plus additional recently developed capabilities. Many additional verification/validation suites have been developed to cover the new ranges of analysis and capabilities.

2 MCNP5-1.60 RELEASE & VERIFICATION

The latest release of the MCNP5 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 [6,7], except where bugs were discovered and fixed. The bug fixes and enhancements are discussed in [2], supplemental pages for the MCNP manual are provided in [3], and verification/validation work is described in [4]. In the sections below, we summarize the code enhancements and provide some results from the verification/validation effort.

2.1 New Features in MCNP5-1.60

2.1.1 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 [8,9].

2.1.2 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 [3], along with input instructions and examples.

2.1.3 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 [3]. 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.

2.1.4 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 *merge_mctal* and *merge_meshtal* utilities, used to merge results from different independent jobs, were updated and made more general. General enhancements were made to the build system, parallel processing efficiency, continue runs, random number generator options, number of nesting levels for universes, etc.

2.2 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.

2.2.1 Verification/validation test suites

Regression - The standard MCNP5 Regression Test Suite [1,4] 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 [10] consisting of 31 problems from the *International Handbook of Evaluated Criticality Benchmark Experiments* [11]. 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 [12] 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 [10,13] 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" [14] 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 [14]. 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 [8,9]. 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 [8,9] 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 [15]. 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 [11].

2.2.2 Verification/validation calculations

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.

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

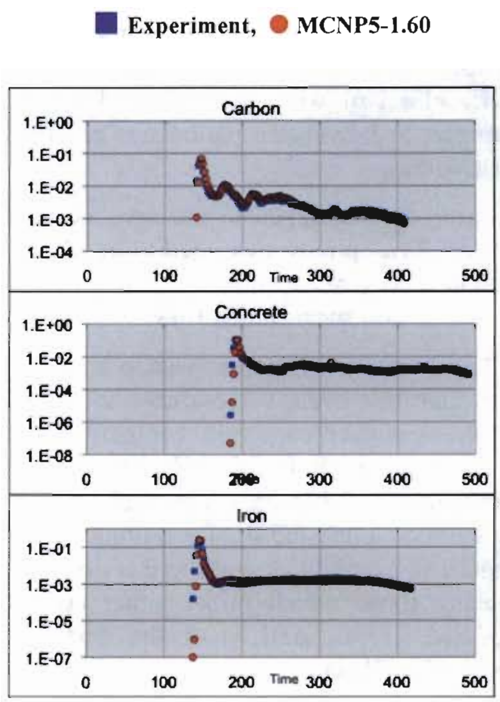
Table II. MCNP Criticality Validation Suite, Results on Mac OS X for ENDF/B-VII.0

	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

Figure 1. Pulsed Sphere Problems



3 MCNP6 DEVELOPMENT

While MCNP6 is simply and accurately described as the merger of MCNP5 and MCNPX capabilities, it is also the result of 4 years of effort by the MCNP5 and MCNPX code development teams (XCP-3 and D-5 groups). The teams have agreed to combine code development efforts to produce the next evolution of MCNP. While maintenance and bug fixes will continue for MCNP5-1.60 and MCNPX-2.7.0 for upcoming years, new code development capabilities will only be developed and released in MCNP6. In fact, the initial beta release of MCNP6 contains 15 features previously not found in either code. The goal of the initial beta release is to begin transitioning experienced users so that they can help perform necessary verification/validation for a wide range of specific applications.

3.1 MCNP5 and MCNPX Merger

MCNP6 was created by merging lines of coding from MCNPX into a local version of MCNP5 which had already been upgraded to use more Fortran 90 features and adapted to transport protons. As the lines of Fortran were taken from MCNPX, conflicts in variable names, array dimensionality and lengths, common blocks, subroutine calling logic, hardwired parameters, default parameter settings, transported particles, input card processing, compilation and build mechanics, and output file formats were resolved. When the conflict was severe enough to cause lengthy delays in the merger progress, or when both codes had independently developed different algorithms for the same capability, those lines of code were identified and wrapped with a flag to preserve each of the parent code's methods. This flag can be set in the MCNP input file using the *dbcn* input card. As MCNP6 continues to be prepared for a production release, these issues will be resolved and the *dbcn* options will be removed. Duplicate capabilities will be evaluated, and one algorithm will be deprecated or given its own input card or keyword. These changes will be implemented to have minimal, if any, impact on the input file.

During the merger process, meticulous care was taken to maintain the confidence in the code's calculated results. Throughout the merger process, MCNP6 was frequently run before and after each specific set of changes (occasionally even single line changes) to isolate and understand the specific effect of what was being changed. Even changes as simple as converting 4-byte real parameters to 8-byte real parameters can be detected in the regression test suite and isolated from other changes.

Care was also taken to preserve as much backward compatibility for input files as possible, although *dbcn* options may need to be added to some MCNPX input files to run with MCNP6. As in previous code releases, there is no expectation that MCNP6 can read MCNP5 or MCNPX binary files, such as *runtpe* or *htape* files.

The intent of the merger was to create a new code with the existing capabilities of each code. While that has been successfully completed, there has been only modest effort to make all capabilities of each code fully compatible with every other capability. In fact, this would constitute new development and will likely be proposed to sponsors in the future. An example of this is the preservation of MCNP5's OpenMP shared memory threading, which enables using multiple processors on a desktop PC for a single execution. MCNP6's OpenMP capability will work will all the MCNP5 capabilities, but there is no expectation that they will work with MCNPX capabilities, especially those which utilize other code packages, such as the high energy models (CEM, LAQGSM, INCL, ABLA) or the delayed particle emissions (LLNL's photon multiplicity or LANL's CINDER).

3.2 MCNP6 New Features

3.2.1 Adjoint-based perturbation theory

MCNP6 contains the first implementation of adjoint-weighted tallies for perturbation theory in continuous-energy Monte Carlo. The adjoint-weighted tallies are implemented using the iterated fission probability [8], similar to the MCNP5-1.60 approach to determining adjoint-weighted reactor kinetics parameters.

Starting from the neutron transport equation and applying a first-order perturbation, the following expression for the change in reactivity ρ can be derived: $\Delta\rho = \langle\psi^{\dagger}, P\psi\rangle / \langle\psi^{\dagger}, F'\psi\rangle$ The reactivity is related to k in the typical way, $\rho = (k - 1)/k$. The angular flux is ψ and its adjoint is denoted by $\psi^{\dagger}$. P is the operator for the perturbation taking the form: $P = \Delta\Sigma_t - \Delta S - \lambda\Delta F$. The eigenvalue $\lambda = 1/k$, and the three terms from left to right, are the change in the total cross section, the change in the scattering operator, and the change in the fission multiplication operator. F' is the perturbed fission operator. Using adjoint-weighted perturbation theory [8], MCNP6 can compute reactivity changes that can be used to calculate sensitivity coefficients of k with respect to some cross sections. Monte Carlo techniques are used to determine the numerator and the denominator in a continuous-energy forward calculation and the change in reactivity can be estimated by taking the ratio.

3.2.2 Geometry mesh file creation and read

MCNP6 provides the initial file-based link to the LANL discrete ordinates neutron and photon code Partisn, separately distributed by RSICC. The initial intent is to provide an easy way to perform Monte Carlo vs. SN comparisons, separating geometry, multigroup data and methodology effects. The longer-range goal is to be able to take the adjoint flux weights from Partisn to use within MCNP for weight windows. The initial capability takes MCNP's combinatorial solid geometry, creates a homogenized regular mesh of materials in 1D (r), 2D (rz, xy) or 3D (xyz), and writes a Partisn-style geometry file, as well as reads a Partisn-style geometry file for continuous energy neutron transport.

3.2.3 Low energy photon transport for atomic cross sections

MCNP6 has extended the minimum energy cutoff for photon transport down to 1 eV. The necessary photo-atomic cross sections from ENDF/B VI release 8 are included in an interim photo-atomic library that users can select. The default photon energy cutoff remains 1 keV, so the user must explicitly request a lower cutoff. These lower energies can be specified on the source, dose response function, and energy bin cards. While they are likely compatible with other energy-specific cards, not all possible combinations have been tested. Users are cautioned that at very low energies, molecular and other effects become important for scattering and absorption, and these more complex effects are not yet included in the photon transport methods. In addition, electron transport has not yet been extended to these low energies.

3.2.4 Complete photon-induced atomic relaxation

Complete element-specific relaxation processes, with the emission of fluorescent photons and Auger and Coster-Kronig electrons, can now be modeled in MCNP6. Again the necessary data (from ENDF/B VI.8) are included in an interim library that users can specify. Going beyond previous MCNP treatments, which considered only K-shell and average L-shell transitions, the new treatment addresses the full detailed relaxation cascade, sampling all allowed transitions down to the photon and electron energy cutoffs, and providing a much more detailed prediction of the relaxation spectra. It should be noted that higher-order effects in which early transitions change the probabilities of later transitions in the same cascade are not modeled, and that relaxation from electron-induced atomic vacancies has not yet been implemented.

3.2.5 Explicit tracking of electrons and light ions (d, t, ^{3}He, ^{4}He) in magnetic fields

Particle tracking in magnetic fields has been added to MCNP6. Two methods have been implemented:

1. Use of magnetic field maps calculated by the COSY Infinity code [16]
2. Direct tracking in a magnetic field defined in the input file. Currently, only constant and dipole fields are available.

The *bfld* card can be used to model magnetic fields that co-exist with materials (such as air). This capability is an alternative to use of the COSZ maps, which can only track particles in a vacuum.

3.2.6 Nested *dxtran* spheres

dxtran spheres can now be nested inside of each other. The nesting is reasonably general. For example, more than one *dxtran* sphere may be nested inside a larger *dxtran* sphere and the nested *dxtran* spheres need not be concentric. The primary restriction is that the spherical surfaces must not intersect. This nesting allows *dxtran* particles to be directed to one or more regions of interest.

3.2.7 Uncollided secondaries

An uncollided particle in MCNP was historically defined to be any particle that had not undergone a collision since its creation as a source particle or as a secondary particle. This definition, in which secondary particles are created as uncollided particles, makes separation of the contribution from the direct source and contribution from secondary particles difficult for the user. This is especially true when users employ track-length tallies in radiography applications instead of next-event estimators. A new cell card has been added to MCNP6 that allows the user to control if secondaries are born as uncollided or collided particles.

3.2.8 Time bins for mesh tallies

Time bins have been added for the MCNP5 style mesh tallies. Users can specify time bin boundaries in units of shakes (1 shake is 10^{-8} sec) on the *fmesh* card. The tally results can be obtained as integrated over the time bin (units of cm^{-2}), as an average rate (tally per unit shake), or as a tally per unit energy (MeV^{-1}). Specific *fmesh* time bins can also be plotted in the mesh tally plotter.

3.2.9 Enhanced photon form factors

New form-factor data from ENDF/B VI.8 for coherent and incoherent photon scattering are available in an interim photoatomic transport library that users can select. These data extend the treatment of coherent and incoherent scattering to higher energies and/or larger scattering angles. The interpolation algorithms for the form-factor data have also been corrected for validity over the enhanced energy/angle range. These improvements provide a more complete representation of photon scattering, and are especially important for backscattering of coherent photons.

3.2.10 Electron energy-straggling improvements now default

The "detailed straggling logic" for the application of Landau theory to the sampling of electron energy-loss straggling is now the default behavior of MCNP6. This method provides a more realistic prediction of the electron energy-loss distribution, and eliminates many of the stepsize artifacts exhibited by the previous two methods, which remain optionally available for backward compatibility or study of earlier results.

3.2.11 Surface and cell flagging now possible with MCNP5 style mesh tallies

Mesh tallies can be used in combination with the surface (*sf*) and cell (*cf*) flagging tally cards. However, unlike the regular tallies, only one mesh tally, the flagged tally, is created. A separate mesh tally will need to be provided for unflagged tally results.

3.2.12 Upgrade to CEM03.03 and LAQGSM03.03

The LANL high-energy physics models have now been updated to their most recent releases. The stand-alone versions of CEM03.03 and LAQGSM03.03 are also available from RSICC.

3.2.13 Generation of gamma rays from muonic atoms

When a negative muon survives to reach its energy cutoff, it attaches to an atom to form a negatively charged "muonic atom." The muon then relaxes by a series of transitions toward the most tightly bound shell, emitting fluorescent gamma rays, in analogy to the electronic transitions characterizing ordinary atomic relaxation. Both MCNPX and MCNP6 contain a programmed library for muonic gamma-production for a variety of isotopes of interest. A new feature of MCNP6 is the ability to read and sample from new data in independent data files. This is a work in progress, since standard formats for such data files have not yet been developed.

3.2.14 Pre-collision next event estimator

A pre-collision next-event estimator has been developed for MCNP6. It augments the post-collision next-event estimator that has historically been used for point flux estimation in MCNP. The pre-collision next-event estimator includes the contribution of all possible reactions before the collision isotope and resulting reaction are sampled. This has the advantage of providing an improved expected estimate per collision, but with a significant increase in the computational cost per collision. This improved sampling technique removes the requirement to suppress coherent scattering for photon transport problems that include photon next-event estimators. The sampling of all possible scattering reactions generally provides an increase in the Figure of Merit (FOM) for most photon problems. This increase in the FOM can be significant when the contribution to a photon next-event estimator is primarily from forward scattering. For most neutron problems there is not typically a large increase in the FOM. However, for both photons and neutrons the pre-collision next-event estimator increases the convergence rate as measured by the time to pass MCNP's 10 statistical checks.

3.2.15 Double-differential particle interaction cross section generator

MCNP6 allows the application of high-energy nuclear interaction models in a cross section generation mode, without particle transport. A source may be specified inside a medium; each history will consist only of the interaction of the source particle at the source energy with the components of the medium. The tallied outcome from the event consists of the energies and direction cosines of the secondary particles and the recoil nuclei. Although one expects that, in normal applications, the material composition will be a single isotope, averaged results may be obtained for a natural multi-isotopic element or a complex composition.

3.3 MCNP6 Testing

The first release of MCNP is considered a "beta" release, not a "production" release for two reasons: First, many of the *dbcn* flags are still present, preventing full operability of certain features. Second, the traditional extensive verification/validation effort needed for a production level release has not yet been performed. Until the MCNP6 code team has tried this new code in a wide variety applications with comparisons to other codes or benchmarks, the release will be considered a beta release. It is expected that users of this initial release apply MCNP6 to the problems that they know well and have some intuition about, and report their findings to the MCNP6 team, either pro or con. Evidence for appropriate performance of MCNP6 should be added to the MCNP6 documentation and verification test suites, and evidence of discrepancies, especially discrepancies with MCNP5-1.60 or MCNPX-2.7.0, should be submitted for investigation.

A small piece in the overall confidence of MCNP6 is its use of automated regression testing suites. About 900 problem test suites are run nightly on Windows 64, Linux 32 and Linux 64 bit computers, in serial, mpi, omp, and mpi+omp modes, with Intel 10, Intel 11, Portland, Absoft and Gfortran compilers. The serial tests are also compiled with array overflow detection and uninitialized variable checks. The results of these tests (more than 20K test problems) are displayed on a large TV in the XCP-3 lounge area. MCNP6 also has several verification and validation test suites, which are currently run by hand.

4 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).*

Limited beta testing of MCNP6 outside of LANL began in early 2011. A more general beta test period is planned for the Fall of 2011, and then a fully supported production release in 2012. It is expected that all subsequent development and support will be focused on MCNP6, the unified and extended code. End-users in all application areas need to be aware of the forthcoming MCNP6 release and begin planning for the transition to the new code in 2012 and beyond.

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