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RELEASE OF MCNP6.2 & WHISPER-1.1 – GUIDANCE FOR NCS USERS

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ABSTRACT

In 2017, a new version of the MCNP6 Monte Carlo code package was released – MCNP6.2. This is the first version of MCNP to include the Whisper package to support sensitivity-uncertainty based nuclear criticality safety validation. This paper summarizes changes to MCNP6 from previous versions, with emphasis on those changes and new features that are important to NCS practitioners.

Key Words: **Monte Carlo, neutron transport, criticality**

1. INTRODUCTION

The MCNP® Monte Carlo code has been used for high-fidelity analyses of nuclear criticality safety (NCS) problems since the 1970s. In 2017, a new version of the MCNP6 [1,2] Monte Carlo code package was released – MCNP6.2 [3] with ENDF/B-VII.1 nuclear data [4]. This is the first version of MCNP to include the Whisper [5] package to support sensitivity-uncertainty based nuclear criticality safety (NCS) validation. This paper summarizes changes to MCNP6 from previous versions, with emphasis on those changes and new features that are important to NCS practitioners.

MCNP6.1 was released in 2013, MCNP6.1.1 in 2014, and MCNP6.2 in 2017. MCNP6.2 provides all of the standard methodology for criticality calculations available in previous versions along with new capabilities. The MCNP6 releases include fully-tested and verified versions of MCNP6 for criticality safety [6,7], the ENDF/B-VII.1 nuclear data libraries, a Reference Collection of over 800 technical reports, and a collection of verification/validation test suites with over 1400 problems.

Whisper is a statistical analysis package developed in 2014 to support NCS validation [5]. It uses the sensitivity profile data for an application as computed by MCNP6 along with covariance files for the nuclear data to determine a baseline upper-subcritical-limit (USL) for the application. NCS analysts may then use this baseline USL from Whisper along with their expert judgment to help set the USL for a range of normal and credible abnormal conditions.

2. NEW FEATURES & CHANGES IN MCNP6.2

MCNP6.2 includes a number of new features not present in previous versions. The features that are relevant to NCS calculations are summarized in this section. While there were more than 300 bugs fixed in going from MCNP6.1 to MCNP6.2, only 3 code-bugs and 3 data-bugs are specific to NCS applications. These bug-fixes and other enhancements are also discussed below.

2.1. New General Features Relevant to NCS

- MCNP6.2 has the same or better performance than MCNP6.1.1, roughly 1.5-2 times faster than MCNP6.1 for NCS applications, and is even slightly faster than previous versions of MCNP5. For NCS applications, significant improvements were made in the energy and cross-section treatment for neutron calculations, the parallel threading performance, and efficient treatment of the checking for the multitude of options available in MCNP6. These improvements have been previously documented in [8].

- For the past 40 years, all of the input for MCNP was limited to lines with a length of 80 characters. This limitation has been removed, and MCNP6.2 permits input lines of up to 128 characters. While this improvement seems trivial, the longer line length permits more spacing of input fields, reduces the number of continuation lines, and can greatly improve the clarity of input files.

- The filenames used by MCNP6.2 may be up to 256 characters in length, and the command-line input may be up to 4096 characters. This permits more descriptive filenames and suffixes.

- During the installation process, a log file records each step in the installation. A separate log file records all steps in the installation testing process. These log files may be retained to provide a complete record of the code installation and testing.

- The Whisper-1.1 package is available, including the Whisper code, supporting scripts, 1101 ICSBEP [9] benchmark problems (with input files and sensitivity profiles), and ACE-formatted covariance files for the nuclear data. Over 50 documents related to Whisper-1.1 are included in the MCNP Reference Collection [10]. The Whisper package provides sensitivity-uncertainty tools that may be used to support NCS validation.

- The suite of analytic criticality benchmarks [11,12] can now be run using the continuous-energy physics treatment, whereas previously these benchmarks could only be run using multigroup physics.

2.2. Changes in Nuclear Data Libraries

The ENDF/B-VII.1 nuclear data files in ACE format are included, along with continuous S(α,β) thermal scattering data, and all older data files are also available. A few datasets in ENDF/B-VII.1 were fixed from previous releases:

- **Revised Nuclear Data for Hydrogen [13]:** The ACE data files for hydrogen based on ENDF/B-VII.1 data that were released with MCNP6.1 and MCNP6.1.1 did not include data for photon production. The ACE files are 1001.80c through 1001.86c. While (n,γ) reactions were properly included in all relevant cross-sections, the specific data for the number and energy of photons produced in the (n,γ) reactions was not included in those ACE files. The updated ACE

files for hydrogen are designated 1001.90c through 1001.96c. These files are identical to the previous hydrogen data files, except that the photon production data is included.

- **SiO_2 S(α,β) Thermal Scattering Data [13]:** The **SiO_2** S(α,β) thermal scattering data released with MCNP6.1 and MCNP6.1.1 was incorrect, due to errors in the ENDF/B-VII.1 data at the time. The ENDF/B-VII.1 errors were corrected, and the ACE files for **SiO_2** S(α,β) thermal scattering data were regenerated. The previous data, ACE files sio2.30t through sio2.36t, are incorrect and should not be used. The new replacements, sio2.10t through sio2.16t, should be used instead.

- **Zirc-Hydride S(α,β) thermal scattering data at 1200K [14]:** The ACE file for thermal scattering in hydrogen at 1200K released with MCNP6.1 and MCNP6.1.1 was incorrect. The errors were corrected, and a new datafile is included with MCNP6.2. Specifically, ACE file h-zr.27t is incorrect and should not be used; ACE file h-zr.28t is the replacement with corrected data.

- **New Listing of Available ACE Data [15]:** The report listing all of the ACE datasets available with MCNP6.2 was updated. This reference should be used in place of previous listings to ensure that the proper ACE data files are used in NCS calculations.

- **New default XSDIR file for MCNP6.2:** The XSDIR file used by MCNP is a datafile containing available ACE files, with the preferred (default) files listed first. MCNP5 and previous versions used a file named *xsdir*. MCNP6.1 and MCNP6.1.1 used a file named *xsdir_mcnp6.1*. MCNP6.2 uses a file named *xsdir_mcnp6.2*. While *the xsdir_mcnp6.2* file can be used with any of the MCNP6 versions, it should not be used with MCNP5, since the default thermal scattering treatment is continuous (which was not correctly handled by MCNP5).

2.3. Changes in MCNP6 Coding

- **Fortran compiler:** The production versions of MCNP6 have been compiled using the Intel Fortran compilers and the gcc compiler for C/C++ portions of the code. MCNP6.1 and MCNP6.1.1 were built using Intel Fortran Version 12, while MCNP6.2 was built using Intel Fortran Version 17. 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 round-off between the compilers. Extensive testing with realistic NCS problems was performed to ensure that compiler differences and other coding changes did not affect the validity of NCS calculations [7,8,9].

- **Compliance with Fortran 2003 International Standard:** All of the MCNP6.2 source coding was reviewed and corrected if needed to ensure that MCNP6.2 Fortran coding is 100% compliant with the Fortran 2003 international standard. In addition, procedures for building MCNP6.2 executables from the source coding were revised to require that all Fortran coding adheres to the standard and that standards-checking is always performed by the compilers.

- **Software Quality Assurance:** MCNP6.2, Whisper-1.1, the MCNP Reference Collection, and the MCNP data files are all maintained under strict SQA procedures. All coding, data, and test problems are maintained using the *git* code management tools and the TeamForge configuration management suite for tracking all modifications, changes, and documents.

- **Warning issued if the neutrons/cycle is too small:** For the past 10 years or so, the MCNP developers have presented recommendations on "best practices" for NCS calculations in MCNP classes, conferences, and university classes [16]. One of the recommendations has been that at least 10,000 neutrons/cycle be used in all NCS calculations to avoid k_{eff} bias from the renormalization that occurs each cycle in the numerical iterations. MCNP6.2 checks that the number of neutrons/cycle is 10,000 or greater, and issues a warning message if that condition is not true.

- **Continuous S(α,β) numerics**: Regarding bug fixes, MCNP6.1 had a small, infrequent error in dealing with the continuous-energy S(α,β) data: For some S(α,β) 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. 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 use the same (corrected) coding for S(α,β) thermal scattering, so should give the same results.

  After the release of MCNP6.1.1 with the S(α,β) fix, additional problems were found with round-off errors for certain S(α,β) datasets. In particular, the zr-h.20t and zr-h.30t data. In the continuous-energy sampling scheme for the exit energy, random sampling is performed for a linear probability density, requiring a square root. For some sequences of random numbers, round-off problems led to improper cancellation and the square root of a negative number. For MCNP6.2, additional checks on this round-off were introduced, and if needed the sampling is performed by a different, robust method that avoids the negative square roots. Since this round-off problem was extremely rare, the different robust method is only used if needed. In nearly all cases, the previous method works correctly. This hybrid approach was taken to avoid changing the random number usage for all MCNP problems. Only the rare problems affected by the round-off error use different random number sequences, hence verification-validation testing is unchanged except for a very few cases.

- **Coincident surface treatment:** The *universe* and *fill* concepts were introduced into MCNP in the late 1980s. That is, when defining a cell in MCNP input, the cell can be filled with a universe rather than a single homogeneous material. We will refer to the cell being defined and filled as a *container* cell. A universe is a collection of cells (tagged with the same *u=n* universe number *n*). The problem encountered with the original universe/fill treatment occurred when a bounding surface of one or more cells in a universe was coincident with one of the container bounding surfaces. When this occurred, MCNP sometimes made a wrong decision on which surface a particle had hit (i.e., in a universe cell or the container cell), and lost particles or silent errors were the result.

In the early 1990s, a "fix" for the coincident-surface problem was introduced, first appearing in the release of MCNP4C in 2000. Unfortunately, that fix was flawed. It relied on preprocessing the bounding surface data for all cells and only considered coincident planes, but did not account for possible rotations that can be specified for filling a container with a (rotated) universe. Thus, if a universe was rotated on-the-fly during tracking when filling a container cell, then lost particles or silent errors could be produced. By accident, the coincident-surface fix worked correctly for 0^o and 180^o rotations, but was incorrect for all other rotations. There was also an absolute tolerance of 0.0001 cm used in the scheme for selecting the surface that was hit. (The tolerance could be changed by the *dbcn(9)* input entry.)

For MCNP6.2, the coincident surface treatment was revised. Preprocessing to search for possibly coincident surfaces was eliminated. Instead, all planar surfaces are flagged as possibly coincident. During tracking in a cell contained in a universe, the distances to the bounding surfaces at all universe levels are examined, and the minimum distance is retained. Each distance has an associated level or depth, with level=0 the "real world," level=1 the next deeper universe in the geometry hierarchy, level=2 next deeper, etc. Then, to allow for round-off in the distance calculations, starting at the smallest depth or level (closest to 0), distances are examined in order of depth to see if they are within a relative tolerance of $\pm 10^{-6}$ from the minimum distance. If so, that distance is the one selected, and the remaining distances are ignored. A relative tolerance of $\pm 10^{-6}$ is entirely plausible and consistent as an estimate of possible round-off in the distance calculations that are performed using 53-bit-precision IEEE standard arithmetic. Retaining the smallest distance (within the round-off tolerance) at the least-deep level is what is desired. Note that this distance may actually be larger than the distance at a different (deeper) level, but is the correct logical choice given arithmetic round-off. This choice prevents the selection of an incorrect surface distance.

The newly revised coincident-surface treatment is the default for MCNP6.2, with a default relative tolerance for distance round-off checking of $\pm 10^{-6}$. The older, flawed treatment can be used instead if desired, by setting *dbcn(100)* to a nonzero value. If the older treatment is used, the default for round-off checking is an absolute distance of 0.0001 cm. For either the new or old treatment, the default for checking distance round-off can be overridden by setting *dbcn(9)*, to a relative value for the new treatment or an absolute value in cm for the old treatment.

It is unavoidable that some, but not all, problems that use the universe/fill capabilities will show different results with the new coincident-surface treatment versus the old one. This is due to the different approaches to dealing with arithmetic round-off in the distance calculations. The new coincident surface logic prevents errors when rotated fills are used and is the preferred treatment. In our testing experience, both new and old treatments gave the same results within statistics for all problems that did not involve rotated fills. For problems with rotated fills and coincident-surfaces, the new approach was correct, and the old approach was incorrect.

The use of the *dbcn(100)* option to choose between old and new coincident-surface treatments is provided for a limited time, to permit users to run a problem either way for verification purposes. It is likely that this option will be removed in the next future release (after MCNP6.2).

- **Removal of limit on boundary-list entries for cell descriptions**: In defining cells (regions) in the MCNP input, part of the input is a list of bounding surfaces, with + or – to indicate sense and possible parentheses and union operators. In very old versions of MCNP, the length of the surface list (including operators) was limited to 999 entries. Over the years, this limit was raised occasionally, and was 9,999 in MCNP5-1.60, MCNP6.1, and MCNP6.1.1. Nevertheless, a number of users had complex geometry where larger limits were needed. In MCNP6.2, this limit (involving the internal variable *mlgc*) was entirely eliminated. MCNP6.2 examines the problem specifications and dynamically determines the space required for handling the boundary-list information.

- **k-adjoint first k-effective estimate:** During the calculation of the adjoint-weighted reactor kinetics parameters, MCNP computes an estimate of K_{eff} based upon the K_{eff} in the iterated fission probably method block. The way this was originally implemented, the block K_{eff} estimate was initialized at the end of the block after the first adjoint-weighted tally scores were made. Consequently, the first estimate of these tallies utilized K_{eff} information from the inactive cycles introducing a small bias. Shortly after the MCNP6.1.1 official release, the coding for this was fixed, with the block-estimate of K_{eff} now initialized at the beginning of the block.

  This bug fix does change the results of the adjoint-weighted calculation of the reactor kinetics parameters. However, this change is very small, generally much smaller than the statistics of the tallies computed. In the case where a user is generally conservative when setting the number of inactive cycles, by discarding more cycles than necessary (even just a few), this bug fix has no impact on the quality of the results.

3. GUIDANCE FOR NCS PRACTITIONERS

NCS practitioners should be aware of the following items related to changes in MCNP6.2, relative to the previous versions MCNP6.1 and MCNP6.1.1:

- MCNP6.2 includes 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. Only a few minor bug-fixes or enhancements were made to MCNP6.2 compared with previous versions, and these were extensively verified.

- MCNP6.2 was thoroughly verified against previous versions. In very many cases, results from MCNP6.2 will match exactly results from MCNP6.1 or MCNP6.1.1, and in some cases results may differ but agree within combined statistical uncertainties. All things considered, MCNP6.2 results are as reliable or more reliable than any previous release of MCNP.

- An immediate benefit of using MCNP6.2 (rather than MCNP6.1) is that the new version is typically 1.5-2 times faster.

- NCS practitioners should be aware of the few instances where ACE data files were corrected and new versions released. Calculations involving zirc-hydride should be checked to determine whether erroneous data (described above) were used. Coupled neutron-photon calculations

should also be checked to determine whether they would be affected by the previous lack of photon production data for hydrogen (described above). Calculations involving SiO_2 at high temperatures should also be checked.

- The coding changes to MCNP6.2 physics are relatively insignificant. Corrections to the S(α,β) thermal scattering numerics are generally negligible relative to problem statistics (or, in rare cases, prevent aborts). Similarly, the changes to adjoint-weighting for computing kinetics parameters may result in small differences, generally negligible compared to problem statistics.

- The change to the MCNP6.2 geometry treatment to correctly handle coincident surfaces in problems with *universe/fill* features will produce different round-off in the geometry tracking. This will produce differences in results relative to previous versions, but those differences should be small relative to problem statistics, and are not a concern. Any large differences that arise are an indication of previous (undetected) errors in older versions of MCNP. If any such cases are found, NCS practitioners should not hesitate to contact the MCNP developers for assistance in further diagnosing the differences.

- It is standard practice for NCS work that only validated computer codes, data, and computer systems be used. In verifying and validating MCNP6.2, NCS practitioners should carefully consider and review the verification-validation work reported by the MCNP developers, as well as the updates to the ACE nuclear data libraries.

NCS practitioners are encouraged to install and test the new release of MCNP6.2, with a goal of adopting it as soon as practical. Note that the last version of MCNP5 was released in 2010, and MCNP6.1 was released in 2013. Due to resource limitations, versions of MCNP that are more than 5 years old are no longer supported by the MCNP Team at LANL.

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