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Release of MCNP6.2 & Whisper-1.1 – Guidance for NCS Users

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Release of MCNP6.2 & Whisper-1.1 – Guidance for NCS Users

- Introduction
- New General Features Relevant to NCS
- Changes in Nuclear Data Libraries
- Changes in MCNP6.2 Coding
- Guidance for NCS Practitioners

Introduction

- **2017 is the 70th anniversary of the first Monte Carlo code for particle transport**
  - John von Neumann created the first MC code in 1947 for LANL
  - Targeted the Eniac, actually ran in 1948

- **2017 is the 40th anniversary of the MCNP code**
  - The roots of MCNP extend back to von Neumann's original MC code

- **Recent RSICC releases of MCNP**

MCNP5	– 2003-2013, R.I.P.
MCNP6.1	– 2013, production version
MCNP6.1.1	– 2014, same criticality, faster, beta features for DHS
MCNP6.2	– 2017, includes Whisper code & benchmarks

When? Any day now. Endless delays in completing documentation.

Would like to have the MCNP User Manual on the web, rather than a controlled publication

New General Features Relevant to NCS

- **MCNP6.2 performance**
  - **1.5 – 2 times faster than MCNP6.1 for NCS applications**
  - **Slightly faster than MCNP6.1.1 and MCNP5-1.60**
- **Longer line-length for input files**
  - **Up to 128 characters per line** [80 character limit for previous 40 yrs]
  - **Can improve clarity of input files**
- **Longer filenames & command-lines**
  - **Filenames can have up to 256 characters**
  - **Command-line can have up to 4096 characters**
- **Logfile for installation & testing**
  - **Logfiles to document MCNP6.2 & Whisper-1.1 installation & testing**
- **Analytic Criticality Benchmark Suite**
  - **Now continuous-energy, not multigroup**
  - **Exact results for testing MCNP6.2 criticality algorithms**

Whisper-1.1 Release

- **Whisper-1.1 code**
  - **Upgrade: Whisper-1.0 (2014) to Whisper-1.1 (2016), Total, thorough line-by-line code review - no bugs found**
  - **General performance improvements (threading)**
  - **Portable to Linux, Mac, Windows**
- **Utility scripts for ease-of-use (Linux, Mac, Windows)**
  - **whisper_mcnp.pl – setup & run MCNP6 for sensitivity-profile**
  - **whisper_usl.pl – run Whisper to get baseline USLs**
- **Covariance data files**
  - **Low-fidelity BLO 44-group data, in new ACE format**
- **1101 ICSBEP benchmark cases**
  - **MCNP input files**
  - **Catalog of sensitivity-profiles for every benchmark**
- **Documentation - 70 reports**

  overview, theory, user manual, release notes, applications, nuclear covariance data, SQA, MCNP6 verification-validation, general references on adjoints/perturbation/sensitivity-analysis

Changes in Nuclear Data Libraries (1)

- **MCNP6.2 release includes ENDF/B-VII.1 nuclear data**
  - **All older data is also still included**
  - **MCNP6.2 & Whisper-1.1 installation takes ~45 GB of disk space**
    - ~37 GB is data – ACE files
    - ~ 5 GB MCNP6.2 – code, tests, V&V suites, Reference Collection
    - ~ 3 GB Whisper-1.1 – code, benchmarks, sensitivity catalog, covariances
- **ENDF/B-VIII.0 nuclear data targeted for release in December 2017**
  - **LANL Data Team is investigating web-based distribution, not DVDs**
- **2 updates:**
  - **New Listing of Available ACE Data - LA-UR-17-20709**
  - **New default XSDIR file for MCNP6.2 - *xsdir_mcnp6.2***
- **3 corrections for data errors, with new ACE files:**
  - **Hydrogen (n,g) production data**
  - **SiO_2 $S(\alpha,\beta)$ Thermal Scattering Data**
  - **Zirc-Hydride $S(\alpha,\beta)$ thermal scattering data at 1200K**

Changes in Nuclear Data Libraries (2)

- **Revised Nuclear Data for Hydrogen**

  - **The ENDF/B-VII.1 ACE data files for hydrogen released with MCNP6.1 and MCNP6.1.1 did not include data for photon production.**
    - **BAD: ACE files 1001.80c through 1001.86c**
    - (n,g) reactions were properly included in all relevant cross-sections, but production data for the number and energy of photons was not included

  - **Updated ACE files for hydrogen**
    - **NEW: ACE files 1001.90c through 1001.96c**
    - Identical to the previous hydrogen data, except that the photon production data is included

  - **LANL testing does not show any differences in results for any of the problems in the Criticality V&V Suites**

  - **Only coupled neutron-photon calculations would be affected**

Changes in Nuclear Data Libraries (3)

- SiO_2 S(α,β) Thermal Scattering Data
  - SiO_2 S(α,β) data released with MCNP6.1 and MCNP6.1.1 was incorrect, due to errors in the ENDF/B-VII.1 data at the time
    - BAD: ACE files sio2.30t through sio2.36t
  - The ENDF/B-VII.1 errors were corrected
    - NEW: ACE files sio2.10t through sio2.16

- Zirc-Hydride S(α,β) thermal scattering data at 1200K
  - ACE file for hydrogen S(α,β) at 1200K released with MCNP6.1 and MCNP6.1.1 was incorrect.
    - BAD: ACE file h-zr.27t
  - The errors were corrected
    - NEW: ACE file h-zr.28t

Changes in MCNP6.2 Coding (1)

- In going from MCNP6.1 to MCNP6.2:
  - 1.5-2 times faster than MCNP6.1
  - Long input lines & filenames
  - Important changes for developers & SQA:
    - Fortran compiler
    - Compliance with Fortran 2003 International Standard
    - Software Quality Assurance
  - Non-numeric changes:
    - Warning issued if the neutrons/cycle is too small
    - Removal of limit on boundary-list entries for cell descriptions
  - More than 300 bugs were fixed, but only 3 are relevant to NCS applications:
    - Continuous S(α,β) numerics
    - k-adjoint first k-effective estimate
    - Coincident surface treatment

Changes in MCNP6.2 Coding (2)

- **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**
    - MCNP6.2 was built using Intel **Fortran Version 17**
- **Compliance with Fortran 2003 International Standard**
  - **MCNP6.2 source coding is now 100% compliant with the Fortran 2003 international standard.**
  - **In addition, standards-checking is always performed by the compilers for every build of MCNP6.2**
- **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.**

Changes in MCNP6.2 Coding (3)

- **Warning issued if the neutrons/cycle is too small**
  - **For the past 10 years, the MCNP developers have presented recommendations on "best practices". One of them:**
    - **Always use at least 10,000 neutrons/cycle in NCS calculations**
    - **Avoids nonconservative k_{eff} bias from the renormalization**
  - **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:**

warning. Using <10k neuts/cycle can give significant renormalization bias.

- **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.**
    - Previously, boundary-list length was limited to 999 or 9,999 entries
  - **In MCNP6.2 this limit was entirely eliminated – dynamically determine the memory space needed**

Changes in MCNP6.2 Coding (4)

- **Continuous S(α,β) numerics**
  - **MCNP6.1 had a small, rare error dealing with continuous-energy S(α,β) data:**
    - For some S(α,β) datasets at very low energies (typically 10^{-5}-10^{-4} eV), NJOY lumps together scattering probabilities smaller than 10^{-6}.
    - MCNP6.1 did not handle that properly. Fixed in MCNP6.1.1.
    - Very small differences in a few problems
  - **After the release of MCNP6.1.1 with the S(α,β) fix, additional problems were found with rare round-off errors for certain S(α,β) datasets - zr-h.20t and zr-h.30t. Would result in code crashes.**
    - In continuous-energy sampling for the exit energy, round-off problems led to improper cancellation and the square root of a negative number.
  - **For MCNP6.2, additional round-off checks were introduced, and if needed the sampling is performed by a robust method that avoids 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.

Changes in MCNP6.2 Coding (5)

- **k-adjoint first k-effective estimate**
  - **In the calculation of adjoint-weighted reactor kinetics parameters, an estimate of *Keff* for the previous block in the iterated fission probability method is needed**
    - Originally, the block *Keff* estimate was initialized at the end of the block after the first adjoint-weighted tally scores were made.
    - Tallies for first block used *Keff* information from the inactive cycles, introducing a small bias. Other block tallies OK.
    - Shortly after the MCNP6.1.1 official release, the coding for this was fixed, with the block-estimate of *Keff* now initialized at the beginning of the block.
  - **This bug fix gives small changes in results for adjoint-weighted reactor kinetics parameters.**
    - Change is very small, generally much smaller than the statistics of the tallies computed.
    - If a user is conservative when setting the number of inactive cycles (by discarding more cycles than necessary), this bug fix has no impact on the quality of the results.

Changes in MCNP6.2 Coding (6)

- **Coincident surface treatment (1)**

  - **The *universe* and *fill* concepts were introduced into MCNP in the late 1980s.**

  - **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 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.**

Changes in MCNP6.2 Coding (7)

- **Coincident surface treatment (2)**

  – **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
  - **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.)

Changes in MCNP6.2 Coding (8)

- **Coincident surface treatment (3)**
  - **For MCNP6.2, the coincident surface treatment was revised.**
    - 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.**

Changes in MCNP6.2 Coding (9)

- **Coincident surface treatment (4)**
  - **The newly revised coincident-surface treatment is the default for MCNP6.2, with a default relative tolerance for distance round-off checking of 10^{-6}.**
  - **The older, flawed treatment can be used instead if desired, by setting *dbcn(100)* to a nonzero value.**

    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).
  - **For either the new or old treatment, the default for checking distance round-off can be overridden by setting *dbcn(9)***
    - If the **newer** treatment is used, the *dbcn(9)* value is a **relative tolerance** for round-off checking. The default is $\mathbf{10^{-6}}$
    - If the **older** treatment is used, the *dbcn(9)* value is an **absolute distance** for round-off checking. The default is **0.0001 cm**

Changes in MCNP6.2 Coding (10)

- **Coincident surface treatment (5)**

  - 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.
  - Due to different approaches to dealing with arithmetic round-off in 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 give the same results within statistics for all problems that do not involve rotated fills.
  - For problems with rotated fills and coincident-surfaces, the new approach was correct, and the old approach was incorrect.
  - For problems that do not use universe/fill capabilities, these changes have of course no effect on results

Guidance For NCS Practitioners (1)

- **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**
  - **Only a few minor bug-fixes or enhancements were made to MCNP6.2**
  - **MCNP6.2 was thoroughly verified against previous versions.**
    - Reference: **LA-UR-17-23822** in MCNP Reference Collection on website
    - In very many cases, results from MCNP6.2 will match exactly results from MCNP6.1 or MCNP6.1.1
    - 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 is that MCNP6.2 is 1.5-2 times faster for NCS**

Guidance For NCS Practitioners (2)

- **NCS practitioners should be aware of the few instances where ACE data files were corrected and new versions released.**
  - **zirc-hydride $S(\alpha,\beta)$ data at high temperatures**
  - **(n,g) photon production data for hydrogen, affects coupled neutron-photon calculations**
  - **SiO_2 $S(\alpha,\beta)$ data**

- **The coding changes to MCNP6.2 physics are relatively insignificant.**
  - **Corrections to the $S(\alpha,\beta)$ 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.**

Guidance For NCS Practitioners (3)

- **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.**
  - **Differences in results, small relative to problem statistics, not a concern.**
  - **Any large differences indicate possible (undetected) errors in older versions of MCNP.**
  - **If any such large differences 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 (LA-UR-17-23822), as well as the updates to the ACE nuclear data libraries.**

Guidance For NCS Practitioners (4)

- 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 not supported by the MCNP Team at LANL.