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MCNP 6.1.1 – New Features Demonstrated

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1. INTRODUCTION

For nearly six decades, the Monte Carlo N-Particle (MCNP™) radiation transport code has been under continuous development. In July of 2013, the MCNP 6.1.0 production version [1] was released, which touted over 30 new capabilities since the final releases of MCNP5 and MCNPX [2]. Over the last couple of years, work has been underway on several new features that have been implemented in the 6.1.1 beta version of MCNP [3], which is slated for release in June 2014. Here we discuss these eleven significant features and enhancements and provide sample results for a select few.

2. MCNP 6.1.1 FEATURES & ENHANCEMENTS

In the following paragraphs, we briefly describe the eleven MCNP 6.1.1 beta version features and enhancements, categorized by Geometry (2.1), Source (2.2-2.4), Physics (2.5-2.9), Tally (2.10), and Other (2.11). Due to space limitations, we show results for only a few of these enhancements.

2.1. Unstructured-Mesh Upgrades

The unstructured-mesh transport capability implemented in MCNP 6.1.0 has been extended to include charged-particle transport, non-void background cell, overlap selection by part, integration with DXTRAN and point detectors, and updated tracking algorithms with speedups of 25-50%.

2.2. Cosmic-Source Heavy-Ion Upgrade

The initial cosmic-source feature included the automatic production of protons and alphas, using analytic interplanetary primary spectra, location-dependent rigidity cutoffs, and solar modulation effects. This capability has been extended to include heavy-ion production whenever the user includes heavy-ion transport on the MODE card. The heavy ions currently included in the University of Delaware model are ^{14}N, ^{28}Si, and ^{56}Fe, each of which represents a range of actual cosmic-ray heavy ions. This improvement generally increases the production of secondary particles within the earth's atmosphere.

2.3. Spontaneous-Decay Source Improvements

The spontaneous-decay source option was first implemented in MCNPX in 2008, which accounts for spontaneous-gamma production from radionuclide decay when radionuclide(s) are included in a material (PAR=SP) or specified as a source particle type (PAR=ZZAAA with ERG=0). This capability was extended to include spontaneous neutron and beta production (PAR=SN,SB). A second improvement includes a user specification for the half-life threshold for stability (10th entry on the DBCN card). When the half-life of a radionuclide exceeds this threshold value, it is considered stable (default is 1.5768e16 s). Furthermore, when this stability threshold is increased above its default value, an improved time-bin structure is used to integrate the production time distributions (234 bins instead of 100). A third improvement includes a user specification for the number of decay daughters to include in a decay chain (55th entry on the DBCN card). This improvement included a more effective algorithm for time integration that reduces production errors for long-lived radionuclides to below ~10% [4].

2.4. Release 3 of the Cosmic & Terrestrial Background File

The cosmic-ray source option was implemented in MCNP 6 in 2010, along with the background-source option. This cosmic-source capability was combined with terrestrial radionuclide source modeling to generate ground/sea-level neutron and photon background fluxes on a 5°x10° latitude/longitude grid, which have been incorporated into Release 3 of the *background.dat* file [5]. These spectra can be automatically sampled as a source using the background-source option (PAR=BG,BN,BP with LOC keyword). Improvements over Release 2 data include a refined grid, corrections to the atmosphere model, location-dependent terrestrial component (within US), and increased convergence.

2.5. Light-ion Library Transport

Like MCNPX, MCNP 6 invokes two different physics treatments for particle transport: libraries (or data tables) and models (or event generators). In general, library-based transport offers very accurate collision physics and sampling speed for low-energy interactions (E<~100 MeV) compared to high-energy model-based transport. Since its inception, MCNP has provided library transport for neutrons, photons, and electrons, and with the incorporation of MCNPX several years ago, it also provides library interactions for protons. The light-ion library transport feature extends the proton library-based transport to other light ions, namely deuterons, tritons, helions, and alphas. As with proton library transport, when the incident light-ion energy is above the library maximum energy (E_{max}) it uses model transport, and when the ion energy is below E_{max} it uses library transport. See Fig. 1a for a sample result.

2.6. Correlated Delayed-Particle Production

Delayed-particle production was first introduced into MCNPX in 2006, via a link to the Cinder90 code which produces time-dependent nuclide production/depletion for an entire decay chain. This treatment was recently modified to include an option (SAMPLE=CORRELATE on the ACT card) that invokes Monte Carlo sampling of Cinder90 decay branches, leading to correlated delayed-particle production from a single decay branch. This option significantly increases execution time due to the resampling of every precursor decay (the default behavior saves the production distributions for reuse after the first evaluation) and should only be used when coincidence physics or scoring is necessary.

2.7. Cherenkov Physics

With the extension of low-energy photon physics to 1 eV in MCNP 6.1.0, light production from Cherenkov physics is now possible in MCNP 6.1.1. This is accomplished by user specification of the refractive index of a material (REFI/C/S keyword on the M card) and a charged-particle Cherenkov physics flag (16^{th} entry on PHYS card). When these are specified and the charged-particle's energy exceeds the Cherenkov threshold for that material, visible and ultraviolet photons are created and transported with reflective/refractive effects.

2.8. Delayed-Alpha Production

Following the delayed-neutron/gamma methodology implemented in MCNPX in 2006 and the delayed-beta extension implemented in MCNP 6 in 2012, delayed-alpha production is now included for radionuclide decay [4]. The ENDF/B-V11.1 alpha decay data for 171 nuclides was incorporated into the MCNP 6.1.1 *delay_library_v3.dat* file as a part of this development. This delayed-particle production can be invoked by including the "a" particle type for the NONFISS keyword on the ACT card. Furthermore, a spontaneous-alpha source can be specified using the PAR=SA option on the SDEF card (or PAR=ZZAAA with ERG=0).

2.9. Correlated Prompt Secondary-Particle Production

The library physics treatment, unlike the model physics treatment, suffers from uncorrelated secondary-particle production. While the law of averages is preserved, coincidence physics and scoring is not possible. For example, a neutron can undergo an elastic scatter and yet produce a capture gamma. A library-based remedy to this problem is not really practical as the file size necessary to describe exclusive interaction and secondary-particle production cross sections is prohibitive. New in MCNP 6.1.1, a model physics solution is provided for secondary-gamma production (8^{th} entry on the PHYS:N card) via a link to the LANL-developed Cascading Gamma-ray Multiplicity code [6]. With this option, prompt secondary gammas from neutron interactions are correlated (see Fig. 1b). Work is underway to correlate both neutron and gamma production from neutron interactions, however it is evident that execution speed will be an issue.

2.10. Compton-Image Tally Option

Since the release of MCNPX 2.5.0 in 2005, it has been possible to model coincidence and anti-coincidence of multi-region pulse-height tallies. This capability, called the PHL tally option, feeds standard track-based energy deposition tallies, perhaps combined from multiple particle types, into one or more pulse-height detector regions. In MCNP 6.1.1, this PHL tally option was combined with a Compton-image algorithm, called the COM tally option, to produce a dual-panel grid of Compton coincidences (i.e., Compton image) [7].

2.11. Performance Improvements

Due to the general-purpose nature of MCNP, particle transport speed has steadily decreased over the last several years with the addition of numerous physics and tally enhancements. This trend has been reversed with the implementation of various performance improvements [8]. Examples include the use of logical flags instead of accessor functions for options, in-lining of heavily-used coding, and new hash-based schemes for cross-section energy lookups. These performance improvements make MCNP 6 run faster than either of its predecessor codes (MCNP5, MCNPX) for many problems.

3. CONCLUSIONS

MCNP development continues at a rapid pace to address capability gaps and improvements in algorithms. One geometry upgrade, three source enhancements, five physics features/upgrades, one tally feature, and one other enhancement have been implemented in the MCNP 6.1.1 beta version, set for release in May of 2014, and are discussed briefly in this paper. Work is underway on several additional features and enhancements that will be included in the MCNP 6.2.0 production version, set for release in 2015.

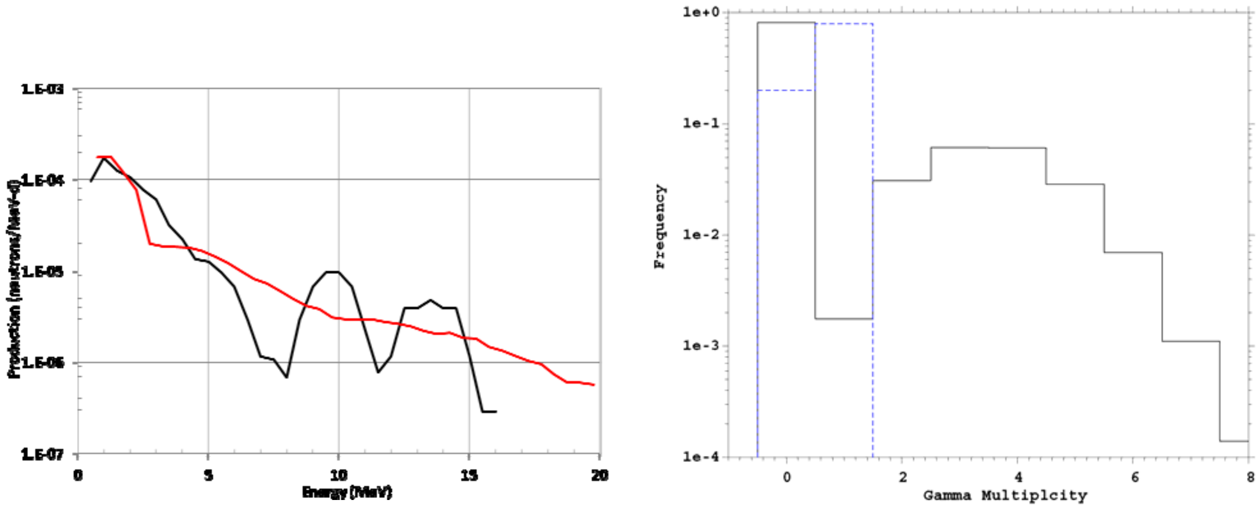

Figure 1. Left plot (a) presents the MCNP 6.1.1 (red) and measured (black) neutron production from 4-MeV deuterons incident on ^{11}B, using a TENDL ACE library. Right plot (b) gives the MCNP+CGM (black) and MCNP+ACE (blue) γ multiplicity distribution for thermal neutrons incident on ^{61}Ni.

4. ACKNOWLEDGMENTS

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5. REFERENCES

1. J. T. Goorley et al., "MCNP6 User's Manual – Version 1.0," Los Alamos National Laboratory report LA-CP-13-00634 (May 2013).
2. J. T. Goorley et al., "Initial MCNP6 Release Overview – MCNP6 Version 1.0," Los Alamos National Laboratory report LA-UR-13-22934 (April 2013).
3. J. T. Goorley et al., "MCNP User's Manual – Version 6.1.1," Los Alamos National Laboratory report LA-CP-14-xxxxx (May 2014).
4. G. E. McMath and G. W. McKinney, "MCNP 6.1.1 Delayed-Alpha Capability," Proceedings of the ANS Winter Meeting, Anaheim, CA, November 9-13 (2014).
5. G. W. McKinney et al., "MCNP6 Cosmic & Terrestrial Background Particle Fluxes – Release 3," Proceedings of the ANS Winter Meeting, Washington, DC, November 10-14 (2013).
6. T. A. Wilcox et al., "MCNP6 Gets Correlated with CGM 3.4," Proceedings of the 2014 RPSD Conference, Knoxville, TN, September 14-18 (2014).
7. G. W. McKinney, "MCNP6 Compton Image Tally Option," Proceedings of the ANS Winter Meeting, San Diego, CA, November 11-15 (2012).
8. F. B. Brown et al., "Verification of MCNP 6.1 and MCNP 6.1.1 for Criticality Safety Applications," Los Alamos National Laboratory report LA-UR-14-22480 (April 2014).