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MCNP™ 6.1.1 - Beta Release Notes

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This document provides an overview of the MCNP 6.1.1 beta release, including the new features, bug fixes and other important changes to how the code runs. The production version of the code, MCNP 6.1, was released in June 2013.

I. Introduction

The latest release of MCNP6 Monte Carlo code is designated MCNP 6.1.1 beta. We recommend that this beta release is not to be used for production level calculations, because it does not have the same level of verification, validation and testing as MCNP 6.1, both in the evaluation of new features and existing feature interoperability, and testing on a wide variety of hardware and operating systems. However, if users wish to perform their own V&V, it is ultimately up to their careful consideration how these executables should be used. This release does have the same high level of confidence for the existing capabilities released in MCNP 6.1.

We have created this release for users interested in testing the new capabilities that are mostly for homeland security and non-proliferation applications. The beta version does not include new capabilities for the criticality safety community, but does run significantly faster than the production version. The MCNP package available from RSICC contains the final production version of MCNP 5 and MCNP X, and the latest production version of MCNP 6, in addition to this beta release and the associated nuclear and atomic data. Additional information on the new features can be found in the associated MCNP references collection, and in several cases, in the revised MCNP 6 Manual.

II. New Features - Code

a. Added Correlated Gamma Multiplicity (CGM) model from LANL, to produce correlated secondary particles (gammas) for ACE-based neutron interactions. This feature also provides more realistic neutron and gamma multiplicities. CGM is invoked by setting the 9th entry on the

phys:n card to 2 (effectively a switch between no/ACE/CGM). The default is still to use ACE data. A test suite (Testing/Features/CGM) was added to test this capability. Artf28690

b. Enabled delayed alphas from nuclear interactions as well as spontaneous delayed-alpha sources (PAR=sa and PAR=zaid on SDEF card). Added delayed-alpha emission spectra to the delay_library_v2.dat file (and higher versions). artf29914
c. Allow spontaneous neutron (PAR=sn)_and beta (PAR=sb) sources. Enable the production of these with heavy-ion decay as well (PAR=ZZAAA ERG=0). Also added DBCN(10), for user input of the half-life threshold for stability (default 1.5768e16 s) Artf27040, artf27488
d. Improved time integration of secondary-particle production from spontaneous decay. Although time-dependence is not used for the sampling of source particles from spontaneous decay, the time-dependent differentials are still integrated to obtain total production values. The linear algorithm used to integrate these complex distributions, that are often spread over many decades in time (e.g., 1e-6 to 1e20 s), can lead to significant errors in the integral values (exceeding 50% in some cases). This improvement reset the decay constants to unity and redistributed the 234 time steps to within 20 s (~10 decays), just for the case of spontaneous decay. User control is provided to allow the user to truncate a decay chain after a certain number of decays (~1s per decay). This integration improvement should keep integration errors to <10%. Artf30049
e. Added correlated sampling of Delayed-Particle Production. This feature offers correlated sampling of delayed particles from spontaneous and induced decay. When chosen, this treatment invokes a Monte Carlo sampling of Cinder90 decay branches. Delayed particle spectra from only the sampled branch are subsequently sampled. Use the SAMPLING=[all|correlate] keyword on the ACT card.
   Three bug fixes involving CINDER_MOD.F90 were also included. Artf28681
f. Several unstructured mesh improvements have been made. Added the capability to use the unstructured mesh geometry with electrons, positrons, and protons (or any heavy charged particle) transport. Previously only neutron and gamma transport were supported. Pulse height tallies, DXTRAN and point detectors now work with the UM. Overlapping models can be selected globally or by part. Background materials are no longer treated as a void, it is the material specified by the container cell. Because of a tracking algorithm change, neutron/photon transport problems have speedups of 20-50%. See the updated UM users' Guide. The code writes version 4 of the eeout file. The um_post_op utility now has the ability to write a single edit to a file ordered by position. The um_pre_op utility can now check element volumes, and check for twisted and deformed elements in the Abaqus.inp file. Artf30091
g. The number of digits in the mctal and output file were increased for large integers. Artf30637
h. Several performance enhancements were implemented. Lines of fortran code were revised to reduce setup and wall-clock runtimes. Includes changes to variable initialization, and binary searches. These improvements are always enabled and there are no user controls for them. Artf30039, artf23878
i. Added the capability to create Cerenkov optical photons from charged particles and have reflection/refraction at surfaces. The keywords refi, refc, refs added to material cards, 16th entry on phys:<pl> card to control/bias Cerenkov production. Default is off. Artf27508
j. Added the Compton Image Tally option, which creates a special tally option (FT card) that enables the creation of two lattice detector grids which can be used in coincidence to create backward-projected Compton circles via a straightforward imaging algorithm. The overlapping of the Compton circles across particle histories should form an image of the source. Artf28594.

k. The Cosmic source feature (PAR=cr) now includes heavy ions. A test suite (Testing/Features/COSMIC) was added to test this capability. Artf29193.

III. New Features – Data

a. The 3rd version of Background.dat file was released and is located in the MCNP_DATA directory. It includes cosmic-source calculations on a 5x10 (latxlong) grid on Earth, and NORM calculations on this grid for the US. This updated file is now the default. Artf28699 and Artf31113

b. The file kcksyst.dat was added to the MCNP_DATA directory. It contains parameter systematics for level density calculations for a wide range of nuclei. It is needed by CoH and/or CGM for poorly known nuclei. The reference for how those systematics were established is: "Phenomenological Nuclear Level Densities using the KTUY05 Nuclear Mass Formula for Applications Off-Stability," T.Kawano, S.Chiba, H.Koura. J. Nucl. Sci. Tech. 43(1) 1-8 (2006)

c. The file ripl-3.dat was added to the MCNP_DATA directory. It is a compilation of all known discrete level data (so low-lying levels) for each nucleus, as evaluated in the RIPL-3 IAEA collaboration effort (https://www-nds.iaea.org/RIPL-3/)

d. Update to the delayed particle emissions library, delay_library.dat, which now includes alpha emissions. The new name is delay_library_v3.dat. MCNP 6.1.1beta will now automatically look for a file named delay_library_v3.dat. artf29914, cmmt124209.

IV. **Code Fixes:** The following is a list of the titles of higher priority bugs that have been fixed since the production release.

artf32748 : Fix for cell-source rejection in unstructured embedded geometries
artf32340 : MCNP6 - fix error messages in LLNL fission package
artf32339 : MCNP6 – bug fix for translation of torus surface
artf31799 : DF dose tally IC=99 option has bug in neutron response
artf31254 : LNK3DNT tracking accuracy bug
artf30048 : Unrealistic scores in segmented electron energy deposition tally.
artf26783 : Time structure of delayed particles contains anomalous structure
artf30637 : Plot and mctal large float and integer
artf31704 : Some problems show xsdir lines printed to screen during initialization
artf31044 : NCIA options not working correctly
artf30139 : Bad Trouble error in acecas
artf31027 : Table 100 print error
artf31263 : FT ROC Tally Option Fails to Rendezvous Properly
artf27841 : WWG Bug
artf31264 : um_post_op misc. fixes
artf30700 : Incorrect creations time of secondary particles from electrons in magnetic field cells
artf31200 : Energy deposition embee gives Nan"s for void cells
artf31180 : DXTRAN diagnostic prints using DD card limits
artf27105 : Magnetic field tracking loses particles if the field direction is perpendicular to a plane surface
artf29785 : Invalid particle termination before tallyd
artf27097 : FT TMC option gives bad results
artf30140 : fixcom bug fix
artf29966 : Fission Multiplicity Crash

artf21940 : DXTRAN diagnotic table incorrect for kcode problems
artf18109 : PWT card and large source weights can produce wrong
artf27742 : Burnup Compatability with Other KCODE Features
artf25705 : Continuous S(alpha,beta) sampling bug
artf28915 : Tally Plots Show Zero Ordinates for Nonzero Tally
artf29432 : Cyclic Time bins created incorrectly from keywords
artf29431 : Cosmic Source Zero Weight Particles
artf29415 : Cosmic Source Option Should Use Provided Polar and Azimuthal Angles
artf29404 : Segfault in expirx print in sourceb
artf29305 : Enable FT ROC with FT PHL
artf29292 : Tracking Differences with MPI and Delayed Particles
artf29205 : Event Log Analyzer bugs & minor fixes
artf18748 : Integer overflow in dxtran diagnotics output
artf29075 : Use of DF 99 Dose option with TMESH tallies is improper
artf28704 : WW MESH keyword "kmesh" doesn not accept degrees or radians
artf28857 : Density-Effect Bug with Mixtures
artf28953 : Conductor Specification Bug
artf28819 : MCTAL Plots For Flux Image Are Often Not Correct
artf28122 : New eprdata does not transport photons at the upper energy limit (100 Ge
artf28646 : particle weight drops without weight cutoff being played when using SI A
artf28599 : Cross Section Plotter Fails to Ignore Coherent Scattering in Some Cases
artf28387 : Setting tags for light ion recoil and aceion
artf31834 : Electron transport hangs in French UM Problem
artf31130 : UM output for regression testing
artf31043 : F8 tallies yield incorrect results with unstructured mesh

V. Changes to Nuclear and Atomic Data

The original S(alpha,beta) data tables for uranium in uranium oxide (u-o2 and u/o2), zirconium in zirconium hydride (zr-h and zr/h), and silicon dioxide (sio2) had some problems in the header of those files. Updated and corrected versions of those files have been provided with a ZAID extension of 3xt; 2xt is the extension of the originally released files. The new (corrected) data tables are for: u-o2.30t ..... u-o2.37t, zr-h.30t ..... zr-h.37t, sio2.30t ..... sio2.36t. These new tables are the default. The following xsdir files have been revised to include these updates: xsdir_mcnp6.1, xsdir_mcnp6.1_endfb-7.0, xsdir_mcnp6.1_endfb-7.1. These files will overwrite the old xsdir files during installation. It is the intent of the mcnp development team to prevent users from using the wrong data tables, so older copies of these files will also be overwritten during the installation of the beta.

VI. Comments on using the Beta release for Criticality Safety applications

MCNP6.1 is the new production version of MCNP [1] released in June 2013. An updated beta version, MCNP6.1.1, is targeted for release in summer 2014 to enable the use of several new features for homeland security and nonproliferation applications. The beta version does not include new capabilities for the criticality safety community, but does run significantly faster than the production version. To verify that both MCNP6.1 and MCNP6.1.1 are performing correctly for criticality safety applications, several suites of verification/validation benchmark problems were run

in early 2014. Detailed results and discussion are provided in LA-UR-14-22480, and summarized here:

The general conclusions from the recent testing of MCNP6.1 and MCNP6.1.1 for criticality safety applications are:

* Both MCNP6.1 and MCNP6.1.1 perform correctly for criticality safety applications.

* While small differences were noted for a few cases, these are strictly due to computer roundoff and are not a concern for verification/validation.

* MCNP6.1 runs roughly 20-30% slower than MCNP5-1.60.

* MCNP6.1.1 runs at least 50-70% faster than MCNP6.1 and 10-15% faster than MCNP5- 1.60.

Criticality safety analysts should consider testing MCNP6.1 or MCNP6.1.1 on their particular problems and validation suites, to prepare for the migration from MCNP5 to MCNP6. It is expected that this migration should be accomplished within the next 1-3 years.

F.B. Brown, B.C. Kiedrowski, J.S. Bull, "Verification of MCNP6.1 and MCNP6.1.1 for Criticality Safety Applications", LA-UR-14-22480 (2014).

VII. Known Issues

The following is a list of known, higher-priority bugs:

artf31853 : Nested dxtran spheres in a lattice caused bad trouble error.
artf28495 : LNK3DNT issues with eigenvalue calculations
artf29933 : Infinite loop in sdef cell sampling in a lattice
artf29268 : Questionable posting to TALMESH and/or TALHEAT manifesting in PHL special tally treatment
artf26747 : Protons on He3 cause array-out-of-bounds error in array XSS
artf28325 : Mix-and-match transport below tabular limits.
artf28042 : mesh tally isotopic production feature results include reactions in a void
artf10665 : Coincident surface errors using tr in fill
artf27093 : Conversion of particle type from LAQGSM to mcnp causes MPI segmentation error
artf18740 : Mesh tally number of tracks calculation incorrect, using FM option -1
artf25475 : lost particles in a magnetic field lattice

VIII. Works in Progress

a. Adding the capability to transport light ion source particles (^{1}H, ^{2}H, ^{3}He, ^{4}He, ^{6}Li, ^{7}Li) onto the same light ion targets, using nuclear and atomic data tables, not theoretical models. The models can be wrong by orders of magnitude for threshold nuclear reactions. This capability is still under development and requires the user to download the nuclear data file (CP2011) and updated xsdir, which will be made available from the mcnp.lanl.gov webpage in the near future. A warning message will be issued by the code if the particle falls below the lowest energy of the

data table. The light ion tables are only for the source particle onto a heavier particle (thus there is no table for ^{7}Li onto ^{2}H). artf27087

b. The charged particle light ion data tables, ACE library CP2011, are not yet available at the time of this beta release, but will be made available shortly on the www.mcnp.lanl.gov website. This data comes from both LANL and TENDL evaluations. See "The Los Alamos CP2011 ACE Format Charged Particle Transport Library for MCNP6", by D. Kent Parsons and Morgan C. White.
c. Correct elevation scaling for the cosmic background source capability is under development.

IX. Changes in running the code.

a. MCNP6 can now print out version information to the screen when the –v is added to the command prompt line. Artf30585

X. Provided Executable Compilation Details

The mcnp v 6.1.1 beta executable for Linux was built with:
Intel Fortran 12.1.5
Gcc 4.7.x
CONFIG= "intel plot omp"
64-bit executable (x86_64 arch)

The mcnp v 6.1.1 beta executable for Linux was built with:
Windows Server 2008 Release 2 Standard – Service Pack 1, with AMD-64 bit CPUs
Intel Fortran 12.1.7
Gcc 4.7.x
CONFIG= "intel plot omp"
64-bit executable (x86_64 arch)

The mcnp v 6.1.1 beta executable for Mac was built with:
Mac OS X 10.6.8 (supported on 10.6 & higher)
Intel Fortran 12.0
gcc 4.2.1
CONFIG="intel plot omp"
64-bit executable (x86_64 arch)

XI. Installing Instructions

The directions for installing MCNP6v1.1 are found in the HTML file "ABOUT_MCNP611.html", located in the top level directory on the MCNP 4th DVD (ie. the DVD specific to the MCNP6.1.1 beta release). If you do not already have MCNP6v1 installed, you need to install it first (using RSICC DVDs 1,2 and 3).