

# LA-UR-13-22900

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Title: MCNP6 version 1.0 Known Issues

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**MCNP6 version 1.0 Known Issues**  
**MCNP6 Development Team**  
 May 29, 2013

This document lists the known issues associated with first production release of MCNP6, MCNP6 1.0. It also lists the known issues with the MCNP5 1.60 and MCNPX 2.7.0 release and their status in MCNP6. High-priority bug fix patches will be made available from the mcnp6 website at mcnp.lanl.gov.

**Issues affecting MCNP6 only:**

*High Priority Bugs in MCNP6*

- 1) Coincident surface errors using *tr* in fill. When using rotations in a fill command, coincident surfaces (after the rotation) are not handled correctly during tracking. Depending on the geometry setup, in some problems particles are lost; in other problems no particles are lost and MCNP gives (silent) wrong answers, in still other problems answers are OK. While this bug results in silent wrong tally results (and thus qualifies for the high priority category), it is not expected to affect many users, only those who use rotated lattice geometries would be affected. Artf10665
- 2) Photon-Electron Physics Improvements (which use the library eplib12) will produce incorrect pulse-height tally (F8) results if used with DXTRAN spheres. Use of the default photon library (mcplib84) does not have this issue. Artf 27942
- 3) When the ACT card keyword DNBIAS (for biasing delayed neutron emissions, not the default) is used in combination with certain fission multiplicity options (FMULT card, keywords METHOD=1 or METHOD=3 (neither the default), the code computes incorrect prompt fission  $\nu$  values results in silent wrong answers. A fix has already been produced and is currently in testing. Artf28074.

*Moderate Priority Bugs in MCNP6*

- 4) Magnetic field tracking loses particles if the field direction is perpendicular to a plane surface. Artf27105
- 5) FT TMC (Time Convolution) option gives bad results artf27097
- 6) Conversion of particle type from LAQGSM to mcnp causes MPI segmentation fault. Artf27093
- 7) DXT fails with LLNL Fission. artf26664
- 8) Time structure of delayed particles contains anomalous structure. Artf26783
- 9) Protons on He3 causes array-out-of-bounds error. Artf26747
- 10) Lost particle in a magnetic field and lattice geometry. Artf25475
- 11) Proton transport can result in lost particles in the unstructured mesh geometry. Artf26974
- 12) Mesh Tally isotopic production feature does not work in void. When using the +fm feature to use each cell's isotopic density for calculating a specific nuclear reaction with a single isotope (specified on a dummy material), reactions are calculated in

void materials. Clearly, no reactions should be occurring in voids. The solution is to use a very low density gas in place of a void. Artf28042

*Selection of Low Priority Bugs in MCNP6*

- 13) HISTP output incompatible with MPI. The HISTP output file does not work correctly with MPI. Each process appears to handle output separately. Routines to handle rendezvous of HISTP information have never been implemented. HISTP also incompatible with threading. Artf27657
- 14) Incorrect source biasing with -31 function. Artf23313
- 15) If the SIn card is after the SPn card, MCNP6 aborts with a fatal error. Please make sure that the SIn card precedes the SPn card. This is understood and is being worked.
- 16) Some instances of irregular detector diagnostics have been observed for the pre-collision point detectors.
- 17) Point Kinetics Continue Runs May Crash with Parallel. On certain systems, crashes have been observed when reading in a runtime file involving Point Kinetics information. This has only been observed for parallel compilations with PGI and is not reliably reproducible. Should this problem occur, users are encouraged to use a different F90 compiler.
- 18) New eprdata does not transport photons at the upper energy limit (100GeV). If the source photon energy is set to 100 GeV, a bad trouble error results. This does not occur if the source energy is reduced to 99.9999 GeV. Artf28122
- 19) Crash during reporting of fatal error. If using the eprdata with both pulse height tally variance reduction and DXTRAN spheres (which should give a fatal error), a format syntax error occurs in the call to erpnt in getxst.F90.

*General Issues in MCNP6 Process or Capabilities*

- 20) Performance Issues. We have noticed that for some cases, MCNP6 takes 50% longer to complete than MCNP5 calculations using the same input file, even though the results produced match exactly. We will investigate this further.
- 21) There are known issues with charged particles on both structured and unstructured mesh geometries. Charged particle transport on standard MCNP geometry (either the CSG or lattice voxels), and neutral particle transport of gammas and neutrons on the structured and unstructured mesh geometries have no known issues.
- 22) For some test problems, a problem run with MPI produces tally results which are not identical to those run without MPI. These appear to be specific to some of the MCNPX model\_based related features. The test cases are: 11 & 12 in Test27a, 05 in Test27c, and 09,13,18,19,20,21 in Tect27e.
- 23) The MCNPX runtime sharing capability for MPI runs with large geometries (ie. many cells) has not been implemented in MCNP6. MCNP6 is able to run in parallel with large geometries in the MCNP5 way, without runtime sharing however.
- 24) The MCNPX 2.7.0 arithmetic tallies capability has not been ported into MCNP6. It is expected that this feature will be incorporated into a future version of MCNP6.

- 25) We have found that some Cygwin command prompts do not recognize control-c interrupts while the native Windows OS on the same machine command prompt does recognize the control-c.

#### *Intentional MCNP6 Merger Decisions*

- 26) There is no listing of code defects (“bugs”) introduced during the merger process. Many of these defects were identified by looking at the results of the >1100 test problems, especially the MCNPX\_Extended test set, but were not documented individually. Most of these bugs have been resolved, but more may exist due to incomplete test suite coverage of the source code. To gain additional confidence in the MCNP6 results, many new Validation tests have been, and will continue to be, added to the MCNP6 test suite. If you have a (preferably published and peer-reviewed) benchmark (with both experimental results and a MCNP input) that you wish to submit to the MCNP6 team, please contact [mcnp6@lanl.gov](mailto:mcnp6@lanl.gov)
- 27) The MCNP6 release does not contain the MCNPX nuclear reaction model (ie. event generator) FLUKA89. There is no intent to incorporate FLUKA89 into MCNP6. The capability to do those nuclear reactions is available in LAQGSM. Artf27113
- 28) The MCNPX style of Pulse Height Tally Variance Reduction (PHTVR) has been removed. The MCNP5 style of PHTVR remains.
- 29) Users who want to use the Bertini event generator must specify it on LCA card. This applies to both transport and the GENXS option on the tropt card, ie. the calculations of the double-differential cross sections.
- 30) The Vacation Matrix method for KCODE problems was removed. This capability

#### **Known Feature Inter-Compatibility Issues**

- 31) Burnup in MCNP6, ported from MCNPX, does not work with many MCNP5 and new MCNP6 features related to criticality. A partial list of those features that do not work together: FMESH, Shannon Entropy, Point Kinetics, Adjoint weighted perturbations and sensitivities for Keff, Fission matrix. Artf27742
- 32) The unstructured mesh geometry is not integrated with all of the pre-existing MCNP features. The full list of known limitations are listed on pg. 18 in the UM User’s Guide (LA-UR-11-05668 Rev 5). A selection of limitations is: limited to only neutrons, photons and protons (although proton transport may result in lost particles), only one UM geometry allowed per MCNP input problem, point detectors, and DXTRAN spheres cannot be in the problem geometry at all, weight windows meshes cannot overlap the UM. Several of these are being worked and are expected to be resolved in the next production release.
- 33) Photon-Electron Physics Improvements (which use the library eprlib12) will not work with DXTRAN spheres and cause PHTRV to disagree with the analog F4 tally. Use of the default photon library (mcplib84) does not have these issues.

#### **Issues in MCNP5 1.60 that are fixed in MCNP6 version 1.0**

These issues are listed as work in progress in the MCNP5 1.60 release notes.

- 1) Incorrect implementation of Doppler photon broadening. With the implementation of Doppler photon broadening in MCNP5, MCNPX and MCNP6 Beta 2, it was discovered that a probability density function algorithm was being used on data intended for a cumulative density function. This results in incorrect sampling of low-energy photon interactions. A updated photon data libraries and a xsdir file has been released on the mcnp.lanl.gov website on the MCNP BUGS page and is included in the MCNP\_DATA directory on the installation DVD. Please note that after the xsdir is replaced, the default photon libraries used have the corrected data. This issue is automatically detected when the data is read and automatically corrected in MCNP6 v 1.
- 2) Windows installation problems with 7z. Several Windows users have reported on the MCNP forum difficulties relating to the self-extraction of the tar files associated with the MCNP5 and MCNP Data releases. This is not applicable, as MCNP6 does not use 7z.exe
- 3) MPI hangs for large calculations. For very large calculations, e.g. > 15K material or >1M cells, some MPI calculations with MCNP5 hang while transmitting the initial problem specification data from the master to the worker processes. This issue has been resolved in MCNP6.
- 4) PERT Card May give Inconsistent Results. Users are advised to exercise caution with the PERT card in MCNP5 v1.60 and earlier when using reaction MT numbers with cross section dependent tallies such as k-effective. All three major known issues were fixed. Artf12037, Artf12993, artf1317

#### **Issues Affecting MCNP5 and MCNPX that are fixed in MCNP6 version 1.0**

- 34) MCNP5/X may crash or give silent wrong answers when trying to sample a particular case with ENDF Law 4. When some of the outgoing energy grids of a particular reaction feature both discrete lines and continua and one or more of the outgoing energy grids of that same reaction only have discrete lines, MCNP will try to sample the continuum as if it were there leading to an error in the sampling. A fix was introduced in MCNP6 that addresses this issue and improves the sampling routines, potentially leading to small differences in answers. For now, this issue appears to be isolated to minor actinides in ENDF/B-VII.1 data, so it should not impact a majority of users. Artf26229
- 35) When point detectors are used with reactions that involve sampling ENDF Law 44 (Kalbach systematics), MCNP will give erroneous contributions to the point detector. This is because the routine for calculating the probability of scattering toward the detector is inconsistent. A fix to this was implemented in MCNP6. Artf26231
- 36) Cell Volume Calculations Incorrect for extreme differences in dimensions. For example, the calculated cell volume of a sphere with radius 0.1 (cm) placed at x=99,999 (cm) is off by a factor of 18. This issue is believed to be caused by roundoff error. Also the order of the cells affected the volume calculation. Artf18745