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*Title:* MCNP5 1.50 Release Notes

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# memorandum

*Computational Analysis and Simulation (X-3)  
Applied Physics (X) Division*

## MCNP5 1.50 Release Notes

This memo serves as a summary of updates to the Radiation Safety Information Computational Center (RSICC) release of MCNP from version MCNP 5.1.40 RSICC to version MCNP 5.1.50 RSICC. Users should obtain MCNP 5.1.50 RSICC directly from RSICC or NEA.

The following sections list the new features, bugs that were fixed, work in progress, and compiler information.

## New Features

### 1. Web-based Documentation

The documentation for MCNP5 has been repackaged and reorganized into an easy to access, web-based format that can be viewed in any web browser. The documentation includes installation notes for Windows, Linux, and Macs; information on the verification testing of MCNP5-1.50; the revised MCNP5 manual; and descriptions of the new ENDF/B-VII data libraries. New sections have been added to include a number of MCNP5 utility programs and an extensive collection of reference documents. This material can be accessed by opening the file `ABOUT_MCNP5.htm` on the RSICC DVD in a web browser.

### 2. Variance reduction with pulse height tallies

Variance reduction for pulse height (F8) tallies is implemented. Allowed variance reduction techniques are:

- Splitting/roulette (IMP card)
- Implicit capture and weight cutoff (CUT card)
- Weight window (WWN card)
- Forced collisions (FCL card)
- Exponential transform (EXT card)
- DXTRAN (DXT card)
- Weight roulette on DXTRAN particle (DD card)
- DXTRAN cell probabilities (DXC card)
- Source biasing (SB card)

- Energy splitting (ESPLT card)
- Time splitting (TSPLT card)

Due to greater increases in the variance, the roulette game may be less useful than for non-pulse height tallies. Although the roulette game is turned on by default for importances (IMP, ESPLT, and TSPLT cards) and weight windows (WWN card), it may be turned off adding "RR=off" on the VAR card. As in previous versions of MCNP, implicit capture and weight cutoffs are turned off by default if a pulse height tally is used in the problem. The only exception is if forced collisions are used, in which case the usual weight defaults are used. However, unlike previous versions of the code, this default can be overridden by explicitly setting the weight cutoffs on the CUT card.

Complete documentation for the theory, MCNP5 implementation, and verification of the pulse height tally variance (PHTVR) feature is provided under the "Variance Reduction" section of the MCNP5 references, accessible from the MCNP5 documentation web pages. This material can be accessed by opening the file `ABOUT_MCNP5.htm` on the RSICC DVD in a web browser.

### 3. New input card: VAR

The VAR card has been added to control variance reduction methods across several variance reduction techniques. Currently, only one keyword is used, RR, which, if set to 'off' or 'no', will turn off the Russian Roulette game for weight windows, and cell, time, and energy importances. This feature could be useful for pulse height tallies.

### 4. Annihilation gamma tracking

MCNP can sample and bank annihilation gammas either from a positron that has slowed down below the energy cutoff and terminates, or from a photon undergoing a pair creation event without the associated banking of a positron (for example when the positron was sampled with an energy below the electron energy cutoff, or in a MODE P problem). Previously, these two situations were treated differently and inconsistently. The resulting difficulties were mostly in bookkeeping, and could be ignored. However, there were subtle errors associated with track-length heating estimators (F6:P tallies) for photons in MODE P E problems, and with "direct" contributions to photon point detector tallies. Furthermore, with the introduction of variance reduction for pulse-height tallies, some of the differences in the annihilation-gamma treatment would have caused serious problems with the variance-reduction algorithm. The code now treats the production and banking of annihilation gammas consistently, more correctly in subtle details, and in a manner that properly supports the pulse-height tally variance reduction algorithm.

### 5. Doppler broadening added to the *makxf* utility code

The *makxf* code is a utility program for manipulating cross-section library files for MCNP5. *makxf* has been used to convert ACE data files between ASCII and binary formats and to make customized libraries containing selected datasets. In 2006, *makxf* capabilities were extended to permit the creation of temperature-dependent libraries. Routines from the NJOY and DOPPLER codes were incorporated into *makxf* to provide for Doppler broadening of resolved data to any higher temperature, and for interpolating  $S(\alpha, \beta)$  thermal scattering kernels and probability tables for unresolved resonance data between two bracketing temperatures. The enhanced *makxf* code

and its new features are fully described in LA-UR-06-7002, "The *makxf* Code with Doppler Broadening", included with the MCNP5 documentation.

## 6. Improved $S(\alpha, \beta)$ thermal scattering

*It should be noted that this feature is experimental and still under development. It is provided in order to enable the testing of a new, improved thermal neutron scattering treatment. The continuous  $S(\alpha, \beta)$  data libraries are not yet part of the standard MCNP library distribution. Users are cautioned that this feature has not received extensive verification/validation, and should generally not be used, except for evaluating the adequacy and accuracy of the new method and data. Production-quality changes to MCNP5 and the MCNP data libraries will occur in the near future, following further testing and documentation.*

The traditional treatment of thermal neutron scattering using the  $S(\alpha, \beta)$  data in MCNP5 involves the use of discrete energy-angle pairs for the neutron exiting a thermal collision. While this treatment is perfectly adequate for the analysis of reactor problems, it is problematic for the analysis of certain experiments (e.g., broomstick problems) where an accurate, continuous treatment of the exit directions is needed.

Recently, both NJOY and MCNP5 have been modified to permit the testing of a new, continuous treatment of the  $S(\alpha, \beta)$  scattering data. MCNP5-1.50 will recognize either the old or the new  $S(\alpha, \beta)$  data formats, without any additional user input.

Bob MacFarlane (the NJOY developer) modified the coding in the NJOY ACETH module to convert the secondary energy distributions from THERMR into pdf/cdf form and pack them into the big inelastic array in the ace thermal file. There is a list of incident energies, a table of the number of points in each distribution, and a table of pointers to the start of each distribution. The data for each incident energy are packed in a way that doesn't quite follow MCNP standards: E', pdf, cdf, cosines, next E', etc. A very small amount of thinning is applied to the distributions by merging energy bins with cdf values that are less than 1e-6.

The sabcol routine in MCNP5 was been modified to read in these new data and use them to drive the sampling. Given an incident energy, the coding finds the closest match in the data. The cdf table is binary searched for the random sample, and the pdf and cdf are used to linearly interpolate for an outgoing energy. The angular distribution is interpolated to this energy. Then this energy is projected up or down to correspond to the actual incident energy along lines of constant energy transfer. This tends to reproduce the sharp break near  $E'=E$  and the various excitation peaks in the thermal data. For lower emitted energies (less than  $0.8 * E$ ), there is a break over to a unit-base scheme to avoid projecting to negative energies. This projection scheme is much faster than real interpolation of incident energy, but it still reproduces things well if there are enough E points in the tables. Once the final outgoing energy has been determined, cosines are sampled from the distribution at the base E and E' before projection. The cosines change more slowly than the energy distribution, so this is reasonable. The sampled discrete cosine is spread out to fill its surrounding cosine values with special measures taken at the edges.

To use this feature, the new continuous  $S(\alpha, \beta)$  datasets must be obtained from the [t2.lanl.gov](http://t2.lanl.gov) website, and version 1.50 or later of MCNP5 must be used. No changes in MCNP5 input are needed. *It is imperative that users carefully check the output file to ensure that the correct data*

are used. Further, the continuous  $S(\alpha,\beta)$  treatment has not yet been extended to cover point detector (F5) tallies; it should not be used in problems with F5 neutron tallies.

## 7. Large lattice enhancements

Several changes in the lattice capability in MCNP5 have been made, due to the recent interest of the medical physics and radiation protection communities in using the lattice capability in MCNP to represent patient-specific CT derived geometries. These changes reduce the amount of memory used, allowing larger problems to be run, and checking to make sure that every filling universe is defined. Specifically, these changes are:

- 1) Splitting the existing lattice variable into 4 separate variables so that this  $3 \times (\text{\#of lattice entries})$  array does not allocate space which is usually not needed for CT-based lattice geometries.
- 2) Ensuring that every universe defined on a `lat=` keyword on a cell has another corresponding `u=` on another cell.
- 3) Reduction in setup times by careful skipping of `chekcs.F90`. Additionally, we have put in place the potential to declare the large lattice array (`laf_fill_u1`) as a 1 byte integer, rather than a 4 byte integer, further reducing memory usage for large lattice problems. As difficulties were encountered passing 1 byte integers with MPI, this feature was not included in the release and must be added through user-compilation in serial or OpenMP mode. Declaring `laf_fill_u1` as a 1-byte integer [`integer(KIND=i1knd)`] also means that all universes (`u=#`) in the MCNP input file must be positive integers less than 255.

## 8. Direct RSSA File Reading for Distributed Multiprocessing

MCNP5 was modified to prevent distributed multiprocessing jobs from unnecessarily sending surface source files via message passing. Previously, all surface source files were sent from the master process to the slave processes via message passing. This feature checks to see if the slave processes can read the surface source files directly. The slaves are only sent the surface source files if they can not read the surface source file from the file system.

## 9. Improve Compton scattering PSC calculation for detectors & DXTRAN

The Hastings approximation to the Klein-Nishina scattering probability density has been removed and the exact formula inserted. The apparent reason for the Hasting's approximation was a concern about numerical computer precision. For the MCNP photon transport energies (above .001 MeV) the numerical computer precision problems do not manifest themselves. The error at .001 MeV is in the ninth significant figure.

## 10. Parse Tabs as Spaces, convert nonprintable chars to blanks

Instead of causing a fatal error, non-ASCII characters in the input file are removed, except for tabs, which are expanded by blanks to the next 8-character tab stop.

## 11. Greater than 8 character File names

All input and output file names in MCNP now have a maximum character length of 256 characters, including path names. Note that file names or path names are still not permitted to contain blank characters.

## 12. Event Log Analyzer (ELA) Utility Code

The Event Log Analyzer (ELA) is a new utility program that works with the revised event log implemented in this code release. See the description of “MCNP Utility Programs” included with the MCNP5/1.50 documentation on the DVD for more information on this product. Details may also be found in LA-UR-06-7796, included in the “utilities” section of the MCNP5 code distribution.

## 13. Utility Programs for Merging Tallies and Mesh Tallies

*merge\_mctal* is a perl script that can be used to combine the "mctal" files created by several different MCNP5 calculations into a single "mctal" file. *merge\_meshtal* is a C++ program that can be used to combine the "meshtal" files created by several different MCNP5 calculations into a single "meshtal" file. See the description of “MCNP Utility Programs” included with the MCNP5/1.50 documentation on the DVD for more information, including LA-UR-08-0249.

## 14. Utility Program for Generating 1-Group Cross-sections

*onegxs* is a C++ program that can be used to create 1-group cross-sections with  $P_0$  or  $P_1$  scattering in ACE format. These cross-sections can then be used to perform multigroup Monte Carlo calculations of analytic benchmark problems. See the description of “MCNP Utility Programs” included with the MCNP5/1.50 documentation on the DVD for more information, including LA-UR-07-4594.

## 15. MCNP5 Random Number Generator

A robust, reliable, stand-alone version of the MCNP5 random number generator is available. It may be used in user-written programs for random sampling of specialized sources, for student exercises in random sampling &/or special-purpose Monte Carlo codes, etc. Updated documentation, source coding, and examples are included with the MCNP5 distribution in the folder utilities/MCNP\_RANDOM. See the description of “MCNP Utility Programs” included with the MCNP5/1.50 documentation on the DVD for more information, including: F.B. Brown, "The MCNP5 Random Number Generator", LA-UR-07-7961 (2007)

## 16. Add additional test suites for MCNP5

The test suites available with MCNP5 have been expanded to include the VALIDATION\_CRITICALITY, VALIDATION\_SHIELDING, and VERIFICATION\_KEFF suites, located in the MCNP5/Testing directory. These include a variety of input files intended to be run for minutes and hours rather than seconds. Documentation on these test sets is included in this distribution.

## 17. Remove tar file input and test templates, replace with text files

The tar files for the MCNP5/Testing/Regression input files as well as the output and mctal system dependant templates have been replaced with individual files in a directory structure. The expected output and mctal templates appear in the Testing/Regression/Templates/Linux and Testing/Regression/Templates/Windows\_NT directories. The Linux templates are used for all operating systems except Windows. The test data libraries have been moved to the Testing/xsec\_data directory.

## 18. OpenMP Threading for All Computer Systems

Over the past year, many Fortran-90 compilers have improved their support for threading on multi-core processors. MCNP5-1.50 fully supports threaded calculations on Linux, Windows, and Mac OS X systems, and can execute using the multi-cores for threaded parallelism. This can result in performance gains of nearly 2X for dual-core processors, nearly 4X for quad-core processors, and nearly 8X for dual quad-core systems. A list of Fortran-90 compilers for each operating system is given below in the section on “Compilers”.

## 19. Installation Script for Linux and Mac OS X Systems

An installation script has been provided for Linux and Mac OS X systems for transferring MCNP5 executables, documentation, source files, testing files, and data library files from the RSICC-supplied DVD to a user's local disk space. This installation script can be accessed from the file ABOUT\_MCNP5.htm on the RSICC DVD in a web browser.

## 20. New Data Libraries for MCNP

The Nuclear Data Team has provided new nuclear data libraries that include ENDF/B-VII.0 nuclear data cross-sections, as well as the older datasets previously available. Documentation for the new files is available from the file ABOUT\_MCNP5.htm on the RSICC DVD.

It should be noted that the new data libraries are large, since the data are provided at several temperatures. As a result:

- *Before installing MCNP5 and the new MCNP Data Libraries on Unix, Linux, and Mac OS X systems, users should make sure that at least 12 GB of free disk space is available.*
- *On Windows systems, additional disk space is required when using the Windows Installer, and users should make sure that at least 25 GB of free disk space is available.*

## Bugs That Were Fixed (sorted by tracker number)

### **1308: SDEF: EXT and RAD as a function of POS does not work** (2005-09-01)

Dependent sources for extent and/or radius as a function of position are now allowed.

### **1317: User notification for perturbations with F5 and F8 tallies** (2005-07-27)

F8 (and F5) tallies do not allow perturbation calculations. Instead of silently giving zero "differences," MCNP now issues a notification both in the perturbation print block and in the tally

fluctuation charts.

**1324: (9439) Source-in-repeated-structures** (2005-07-14)

Index range of 1 in third coordinate (e.g. -1:1 -1:1 0:0 instead of -1:1 -1:1 0) no longer causes a parsing error.

**1328: Check that each fill card refers to a valid universe.** (2006-01-24)

After the input deck has been parsed, MCNP checks to see if the user has accidentally assigned a non-existent universe (a universe with no cells in it) on a fill card. If so, a fatal error is generated.

**1334: Prevent source distribution numbers greater than 999** (2005-09-07)

MCNP does not allow source distribution numbers greater than 999. (See the SIn input card in the MCNP manual.) A fatal error has been added for distribution numbers greater than 999.

**1344: Switched indices for an array used in forced collisions** (2005-11-01)

A bug that caused the forced collision parameter for particle type I in cell J to be confused with that for particle type J in cell I has been fixed.

**1349: Improper use of a lattice in a universe** (2005-12-07)

When a user defines a second cell in a universe with a lattice cell, the maze array is not always filled correctly. A universe with a lattice should not have another cell. A warning message is now printed.

**1350: Errors occur when comments are found after a continuation line marker** (2006-03-21)

A bug that prevented an "&" continuation and subsequent comment on the same line was found. This was fixed.

**1352: Incorrect monodirectional source detector contributions** (2006-03-15)

An error in the planar monodirectional direct source contributions for point and FIR flux image detectors has been corrected.

**1353: Logarithm of zero floating point exception** (2006-09-22)

The mesh tally plotting routine sometimes tried to calculate the logarithm of zero, causing a run-time error.

**1354: Geometry levels and lattice cells missing from geometry plot** (2006-02-24)

An error in the plotting routines that caused the geometry plot to skip some geometry levels and lattice cells was fixed.

**1355: Floating point exception in verification\_keff test suite** (2006-03-16)

For multi-group problems, there was a problem for KCODE calculations where the initial source is over-run and is read again from the srctp file. The values were stored as energy instead of energy groups

**1358: PTRAC printing for test problems** (2006-02-24)

Previously, the code name and version, as well as date and time information, were always printed in ASCII PTRAC files, so that in a regression test ptrac differences could never show a zero result. Now when the MCT parameter on the PRDMP card is negative, as in regression testing, no run-identifying information is printed, so that the difference files can be of zero length if no numerical



differences occur.

**3958: Integer overflow in ptrak.** (2006-04-20)

An integer array receiving 8-byte values was not declared as 8-byte.

**4054: Universe level not checked when a particle leaves a dxtran sphere** (2006-05-09)

The universe level of the current particle was not checked when it left the dxtran sphere, resulting in attempts to take the square root of a negative number.

**4133: Generate an error message for an invalid photon reaction number** (2006-05-18)

Valid photon reaction numbers for FM cards are -1 through -6 and 501, 504, 502, 522, 516, and 301. All other reaction numbers (including 1) produce a fatal error.

**4267: Particle on the outermost weight window mesh boundary number causes indexing errors.** (2006-06-22)

If a particle is on the outermost boundary of a weight window mesh, the wrong index for the wwf array is calculated.

**4269: Integer overflow in ddiag** (2006-06-23)

A 4-byte integer overflow for the number of dxtran energy cutoff score misses was fixed by explicitly declaring a local variable as 8-byte.

**4271: Integer overflow in sourcb** (2006-06-23)

A 4-byte integer overflow bug was found in the sourcb routine that caused execution problems due to low source efficiency. Two local variables were explicitly declared 8-byte integers.

**4351: Array-bounds error associated with ECH() array.** (2006-07-22)

A bug in the allocation of the array that is used for sampling bremsstrahlung angular distribution could occasionally cause (usually negligible) errors and tracking differences between serial and parallel executions of identical problems. The array in question is now properly allocated.

**4441: Variable m3 in subroutine needs to be larger** (2006-07-21)

The value of the variable m3 in the subroutine expunge has been doubled from 1000 to 2000. This change was required to use the new the ENDF/B-VII.0 data libraries

**4541: Out of bounds error for array xss** (2006-08-01)

An array-out-of-bounds error occurred when MCNP tried to expunge data that was not in the original data set.

**4558: FMESH card allows negative values of Z for cylindrical meshes** (2006-08-03)

MCNP now creates a fatal error if negative values are entered for the Z-coordinate with cylindrical meshes.

**4589: Fission source array indexing errors** (2006-08-04)

The index of the fission source array (FS0) could exceed its upper bounds.

**4628: Mesh tally allocation errors** (2006-08-10)

For certain input files, the mesh tally arrays were not allocated properly, causing the code to crash.

**4944: Lost particles due to REC macrobody definition (2006-09-14)**

Particles were being lost since MCNP did not identify all duplicate surfaces in REC macrobody definitions.

**5831: Error in the fission bank during kcode calculations run with MPI (2006-12-12)**

There was an error in the way the fso (fission bank) array was transmitting from the slaves to the master node. This occurred only when the tail of the banked neutrons in the circular buffer ended exactly at the end of the fso array. This resulted in zeros being received (actually NOT received) to the master node. Results in a fatal error during a run and the job aborts.

**5918: Cell-based vs mesh-based weight windows error (2007-01-04)**

Incorrect array indexing of the weight window lower bounds caused incorrect multi-group adjoint sampling.

**6052: Unexpected lost particles (2007-01-23)**

Particles were being lost due to an improper value of JSU in the subroutine knock.

**artf6392: Over indexing of array used to set number of electron substeps. for Avg. Z# > 94. (2007-02-23)**

During problem setup the table lookup of the number of electron substeps for a material with an average Z# greater than 94 caused an array to be over indexed. Increased array to handle Z# up to 100, and logic to prevent over indexing of the array.

**artf6517: Bug in line coloring of postscript plots (2007-03-21)**

Postscript lines were not properly terminated and were being colored by the color assigned to the next item in the postscript file.

**6556: Total user bin not calculated for F8 tallies (2007-03-28)**

MCNP was printing zeros for the results of totals over all user bins with an F8 tally.

**6623: RHP macrobody causes array bounds error (2007-04-04)**

If an RHP macrobody is defined using all 15 input parameters, an out-of-bounds array error occurred.

**6792: Mesh tally array-out-of-bounds error (2007-4-24)**

The use of a DE0 and DF0 cards with mesh tallies caused an array-out-of-bounds error

**6947: Array-bounds error in subroutine crtcze (2007-05-10)**

Faulty logic in the routine that detects excessively-large differences in cell importances or weight windows between adjacent cells could cause temporary array-bounds errors.

**7582: Delayed Neutrons with tme>tco(neutron) result in negative tallies. (2007-07-17)**

Delayed neutrons born after the neutron time cutoff were producing negative tallies.

**8279: Plotting crashes for X-clients with basic fonts. (2007-09-12)**

Basic X11 clients crashed with MCNP when scaled fonts were not available.

**8324: Lethargy Plotting Bug (2007-09-14)**

Error bars for lethargy plots were plotted incorrectly if energy bins were defined below the energy cutoff.

**8472: Wrong cell number printed in the event log** (2007-07-31)

In subroutine surfac, the cell number is set after the call to eventp, causing the wrong cell number to be printed in the event log.

**8994: Doppler broadening not applied to pseudoparticles** (2007-11-08)

Doppler broadening was not applied to dxtran, point, and ring detector pseudoparticles.

**9138: roundoff for tco() initialization & testing** (2007-11-17)

On AIX systems, the time cutoff array, tco(), was not properly initialized in the imcn and nextit routines due to roundoff differences.

**9322: Criteria to determine if the radiography tally is perpendicular to the z-axis too high** (2007-11-08)

The reference value used to test if a rectangular radiography tally plane is perpendicular to the z-axis was changed from 0.99 (cosine of 8 degrees) to 0.999999 (cosine of 0.08 degrees).

**9361: Inaccurate information printed for the FIR tally** (2007-12-17)

The value printed in the outp file for the distance from the origin to the image grid center, was not always correct and is no longer printed.

**9952: Tracking errors when running with MPI and threads** (2007-12-17)

If MPI is used with threading and the CTME card, sometimes an individual MPI process does not run all the histories it is assigned.

**WARNING: Co-existence of Weight Windows with Geometry Splitting**

It is possible for users to be confused over what MCNP is doing when weight window cards (i.e., WWP, WWN, etc.) and cell IMP cards appear in the same input deck.

First and foremost, with the current code implementation, the cell-based geometry splitting and Russian roulette games (IMP games, when played, are only played at surfaces) are not played when either cell-based or mesh-based weight window games are played. The IMP games are not played even if the weight window game is played at collision points and not at surfaces. NOTE: Weight window lower bounds can be determined from the IMP values when SWITCHN on the WWP card is positive, but the restriction still holds.

However, since the weight cutoff game can rely on cell importances, either the default IMP value (default = 1) or the user specified value is used when the weight window in the cell is zero.

When IMP cards are present with the weight window cards, MCNP checks to see if the IMP values differ from 1 and then prints the warning:

"this problem has both weight windows and cell importances."

An additional warning now appears below this warning and says:

"geometry splitting and Russian roulette are not played."

This is intended to tell the users that geometry splitting and Russian roulette are not done at surfaces when there is a weight window present.

## Work in progress

The list below contains items that are known issues with MCNP 5 1.50. Work is in progress to address all of these items.

### **1270: Density Effect Term in Landau Straggling**

In the current version of the Landau energy-loss straggling model for electrons and positrons, the density-effect parameter seems not to be included in the term representing the expected mean sampled value for the dimensionless lambda variable.

### **1287: Parallel calculations of VOV do not agree with sequential runs**

### **1324: Particle tracking bug**

When a source point lies on a surface used elsewhere to define a cell of the problem, that cell seems to be invisible to the source particle, whether the cell is void or filled with a material. Also seen in MCNP4C but the tallies are not zero; a nontrivial number of particles get lost

### **4556: EXT card on a cell line gives fatal error**

If an EXT card is placed on a cell line (ie, the example given on p 3-10 of the MCNP manual) MCNP exits with a fatal error.

### **4654: DXTRAN weight cutoffs**

If electron importances are set to zero in a cell in which the photon importance is not zero, the DXTRAN weight cutoffs are not applied correctly, which can cause in too many particles to be rouletted.

### **5505: Cylindrical Mesh Tally Plotting Error**

In some cases, the cylindrical mesh is not plotted in the correct location

### **5726: Plotting error due to incorrect basis vectors**

The use of the theta and rotate plot commands can cause the plot to be drawn in a left-handed coordinate system

### **7229: Pert card crashes tally plotter**

The tally plotter crashes after reading in a mctal file from a kcode problem with a PERT card.

### **7529: Duplicate IMP items on cell cards not detected**

MCNP does not recognize multiple IMP cards on a cell line as an error. Instead, it used the first instance to set the cell importance.

### **8507: Continuous energy loss ignored for electron/positron track-length tallies**

Track-length tallies for charged particles behave as if an entire step (energy step or angular substep) were taken at a single energy, instead of continuously along the step. This causes artificial oscillations in the energy spectrum for finely resolved energy bins

## Compilers

MCNP5 1.50 has improved support for newer Fortran 90 compilers. The compilers supported are listed below. The gcc C compiler is used for all versions.

The ‘mpi’ notation after a compiler indicates that the compiler can be used to build a parallel, MPI-based executable for MCNP. (Note: In general the same Fortran-90 and C compilers should be used for building MCNP5 as were used for building the MPI libraries [mpich, openmpi, lampi, etc.]. Also, while support for PVM-based parallelism is still available in the MCNP5 build system, that option has not been tested for several years at LANL due to the demise of PVM software on LANL computer systems.)

The ‘omp’ notation after a compiler indicates that threading (also called “shared memory multiprocessing” or microtasking) can be used when building an MCNP5 executable. For computers having multi-core processors (e.g., Intel Core2 duo, Intel quad-core Xeon, etc.), MCNP5 should generally be compiled with the ‘omp’ option. Note that some compilers are not yet suitable for compiling a threaded version of MCNP5.

- Linux (32-bit and 64-bit):
  - Absoft 9.0                      mpi
  - g95 (0.9)                      mpi
  - gfortran (4.4.2)              mpi
  - Intel (9.0, 9.1, 10.0)        omp, mpi
  - Pathscale (3.0)              omp, mpi
  - Portland (6.0, 6.1, 6.2, 7.0) omp, mpi
  
- Windows
  - Absoft (9, 10) \*\*              mpi
  - Compaq (6.6B)                mpi
  - g95 (.91) \*\*
  - gfortran (4.2.1) \*\*
  - intel (9.1, 10.0)            omp, mpi
  - lahey                          mpi
  - portland group (7.1)        omp

\*\* = Plotting is not supported with these compilers.

- Macintosh – Intel-based
  - Intel 10.1                    mpi, omp
  - Absoft 10.1                mpi
  - g95 (.91)                    mpi

- Macintosh – PowerPC-based
  - IBM XLF 8.1                    mpi
  - Absoft 9.2                    mpi
  - g95 (.91)                    mpi
- Sun
- AIX
- OSF1

The reference templates for output and tally files used in the MCNP5 Regression test suite (i.e., installation tests) were generated for Linux and Windows as follows:

Windows:     32 Bit Pentium IV, Windows 2000 Professional SP4, Intel 9.1 f90, gcc

Linux:        64 bit AMD Opteron 2.0 GHz, Red Hat Linux 9, Intel 10.0.023 f90, gcc

For other systems, the Linux reference templates are used. While the MCNP5 developers strive to reduce or eliminate arithmetic roundoff differences that lead to differences in results, users should be aware that compiling and testing MCNP5 with different hardware, operating system, Fortran90 compilers, C compilers, or different build options may lead to differences in results due to computer roundoff. (Results should agree with the reference templates within the combined statistical precision.) For the release of MCNP5-1.50, all of the configuration files for building MCNP5 were changed to make explicit use of the “-r8” Fortran option when compiling MCNP5. The use of this option produces better (but not perfect) consistency of results among MCNP5 executables run on different systems (Windows/Linux/Mac/Unix) or with different Fortran compilers. For more details on this, see the report “Verification of MCNP5-1.50” from the ABOUT\_MCNP5.htm file.

## Installation instructions

Any previous versions of MCNP5 or the nuclear data libraries should be renamed, relocated, or deleted prior to installing the latest versions.

***Before installing MCNP5 and the new MCNP Data Libraries on Unix, Linux, and Mac OS X systems, users should make sure that at least 12 GB of free disk space is available.***

***On Windows systems, additional disk space is required when using the Windows Installer, and users should make sure that at least 25 GB of free disk space is available.***

Installation of the latest release of MCNP-1.50 and the data libraries on Windows systems is the same as described in the PDF file ‘MCNP5 Installation Guide’ that can be accessed from the file ABOUT\_MCNP5.htm on the RSICC DVD.

For Linux and Mac OS X systems, there is a new installation script available, also available from the file ABOUT\_MCNP5.htm on the RSICC DVD.