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*Author(s):* MCNP Team

*Submitted to:* Radiation Safety Information Computational Center (RSICC)  
Oak Ridge National Laboratory,  
Post Office Box 2008  
1 Bethel Valley Road  
Oak Ridge, Tennessee 37831-6171



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## memorandum

*Applied Physics Division*

*Group X-5, Diagnostic Applications*

To/MS: RSICC, Oak Ridge, TN

From/MS: MCNP Team, X-5, MS F663

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### MCNP 5.1.40 RSICC Release Notes

November 2005

This memo serves as a summary of updates to the Radiation Safety Information Computational Center (RSICC) release of MCNP from version MCNP 5.1.30 RSICC to version MCNP 5.1.40 RSICC. No patch file is provided to update MCNP 5.1.30 RSICC to MCNP 5.1.40 RSICC. Users are recommended to obtain MCNP 5.1.40 RSICC directly from RSICC or NEA.

#### Issues

The following items list the new features, bug fixes and minor code improvements implemented in the new release.

#### New Features

##### 1. Lethargy Plots for energy dependent tallies

On the average, neutrons lose a fixed fraction of their energy in each elastic collision with a specific isotope above thermal energies. Lethargy is used in nuclear reactor analysis to assess the average logarithmic energy loss of these elastically scattered neutrons. New to MCNP 5.1.40 are lethargy plots of energy-dependent tallies with a log energy abscissa. These plots are made with the new 'lethargy' plotting command. The area of a tally range under the curve is a measure of the importance of each range to the total. The LOGLIN lethargy plot displays relative contribution of each tally bins by the area under the histogram. See MCNP manual, Appendix B, Section III-F.

##### 2. Logarithmic interpolation for input data

Similar to the linear interpolation input feature 'nI', the capability has been added to MCNP to logarithmically interpolate between two input data values to easily create intermediate input values of equal lethargy. Using the new 'ilog' feature for logarithmic interpolation makes input easier when these types of bins are desired. See MCNP manual, pg. 3-4

##### 3. Neutron Multiplicity

MCNP can now sample the number of fission neutrons emitted from a distribution instead of the previous MCNP method of selecting the integers bounding nu-bar the appropriate fraction of the time. The basis for this neutron physics improvement is that fission neutron multiplicities can be sampled from a Gaussian distribution with a fixed isotope-dependent width. A Gaussian sampling is performed about a value of nu that has been determined for

each fission collision. The sampled value is added to the fission nu for the collision plus one-half. Then the real number is truncated to an integer that is used as the neutron multiplicity. A negative number is set to zero. See MCNP manual, pg. 2-50 and 3-127.

Also included is improved dynamic fission neutron multiplicity output (now Print Table 115). This new output includes factorial moments and neutron multiplicities for the total problem, as well as U-235 and Pu-239 if they are in the problem. Also provided is a check of the sampled average fission nu to the expected average fission nu. From 1 to 3 tables will be printed depending on which fission isotopes are present. See MCNP manual, pg. 2-50.

#### 4. **Stochastic Geometry**

MCNP can faithfully represent millions of 3 dimensional cells using multiple levels of nested geometry, including embedded lattices. To address a strong interest in modeling new reactor technologies where cells can be randomly located, a new feature in MCNP 5.1.40 will allow users to flag selected universes as stochastic that will randomly translate the geometry inside a lattice cell. Particles entering a lattice element containing a stochastic universe will undergo the usual transformations to the lattice coordinate system. Afterwards, additional random translations are made to the lattice cell. Tracking proceeds normally with the universe coordinates fixed until the particle exits the lattice element. See MCNP manual pg. 3-32; LA-UR-04-8668, LA-UR-04-5362.

#### 5. **Source Entropy with Plots**

In criticality calculations, the fission source distribution is presumed to converge and settle before the tallying k-eff. To ensure that tallied quantities are generated by particles sampled from the stationary source, MCNP users have to specify the number of inactive cycles to discard before tallies begin. Relative entropy of the fission source distribution has previously shown to be an effective diagnostic to assess convergence. New diagnostics have been added to MCNP assess convergence of the fundamental mode. See MCNP manual pg 2-180 and 3-77; LA-UR-02-3783, LA-UR-02-6228.

#### 6. **Mesh Tally Plotter**

A new feature in MCNP 5.1.40 is the mesh tally plotter. This feature uses the MCNP geometry plotter to display the mesh tally results and errors superimposed over the problem geometry. The results can be displayed either as a color gradient or as several solid colors, with each color representing a range of values. The user can enter these values as well as the upper and lower limits of the plot. The user can also control which energy bin of the mesh is plotted. In addition, by placing the cursor over a specific mesh tally bin, MCNP will display the mesh tally bin value and relative error on the plot screen. See MCNP manual Appendix B-8 and B-24.

#### 7. **New Electron Energy-Loss Straggling Logic**

For sampling fluctuations in electron collisional energy loss, MCNP relies on a Class I condensed-history algorithm in which parameters of the Landau straggling theory are pre-computed for a standard set of energies and step sizes. During the transport, the Landau straggling distri-

bution is sampled once for each energy step and the resulting energy loss is apportioned over a pre-determined number of smaller angular substeps. This process can be followed using either the "MCNP-style, bin-centered" logic, which remains the default treatment, or the "ITS-style, nearest-group-boundary" logic, which is selected by setting the 18-th entry on the DBCN card to 1. This release of MCNP features a new, more detailed logic in which the Landau distribution is sampled for each angular substep, using the specific energy of the electron and the actual substep size. This approach is still undergoing testing, but appears to result in a more accurate and detailed estimate of the straggling. The new logic is selected by setting the 18-th entry on the DBCN card to 2. See MCNP manual pg. 2-72; LA-UR-05-4404.

## 8. Source Particle Type Specification

The type of the source particle can now be specified on the SDEF card either by particle type number or by particle designator. For example, to specify a neutron source, the user may indicate either "SDEF ... PAR=1 ..." or "SDEF ... PAR=N ...". Similarly, either "PAR=2" or "PAR=P" requests a photon source, and either "PAR=3" or "PAR=E" requests an electron source. See MCNP manual pg. 3-55.

## 9. Positron Sources

In a MODE N P E, or MODE P E, or MODE E problem, it is now possible to specify that a source electron is actually a positron. The user interface on the SDEF card is either "PAR=4" or "PAR=F". Note that this is merely a special syntax, used only on the SDEF card, and does not indicate that the positron is a separate particle type. Positrons are still treated as electrons for purposes of transport physics. See MCNP manual pg. 3-55.

## Minor Code Improvements

- **9933: Speed Tally Enhancement warning message w/ criticality calc**

Frequently criticality calculations use lattices in their geometry. When this occurs, the speed tally enhancement warning message appears, even if there are no F4 tallies, causing unnecessary confusion. This has been fixed.

## Bugfixes

Below are a list of bugs that have been fixed in MCNP 5 1.40. All bugs are tracked and listed by a unique ID number (eg. 6262) in the Sourceforge bug tracker.

- **6262: Terminating Values of the EBD Array (2004-08-10)**

The last value of the EBD array, used to support BBREM biasing of bremsstrahlung photon energy, seems not to be set, and probably should be set to unity.

- **6365: Infinite loop in dopplerp.F90 (2004-09-03)**

The infinite loop is caused by a photon with a low energy and a grazing angle colliding with hydrogen.

- **6575: MCNPLOT crashes when reading in a RUNTPE file (2004-10-12)**

When using the tally plotter, if a second RUNTPE file is read, the code would sometimes

crash with an access violation error.

- **6686: Nonzero relative errors are printed for zero-valued mesh tally bins (2004-10-29)**  
If the ij, ik, or jk mesh tally output format is used and multiple tables are produced, nonzero relative errors may be printed for mesh tally bins that have a zero value.
- **6825: Fix print problem when more t (2004-11-19)**  
Fix print out of integer value when more than 1 million cycles are run.
- **6980: Bug in radiography tallies (2004-12-06)**  
The user incorrectly used an unphysical (negative) value as an input value for the FIR tally. Checks for valid input added to coding.
- **7108: Error in Plotting First Material Total Cross Section (2004-12-21)**  
Problem with the total photon cross-section plot (IXZ option)
- **7194: ANGL not set in function angl (2005-01-10)**  
Variable angl not initialized in function angl, causing floating point error upon return.
- **7291: Multiple DXC card information not used properly in mcnp (2005-01-20)**  
Coding around the DO\_100 loop in celsrf.F90 is not correct when more than 1 dxtran sphere per particle is use.
- **7357: Negative Huge I4KND value in Table 140 (2005-01-27)**  
Values in arrays for Table 140 are forced into the default integer kind which on several platforms is I4KND.
- **7468: Detector diagnostics variables overflowing with nps>2e9 (2005-02-10)**  
Problem with some detector diagnostics output printing negative entries when > 2e9 particles are run.
- **7501: Trouble in itally li>1+lit (2005-02-18)**  
Problem with converting input data from column format to horizontal format and also process the input file information contained on the cell cards.
- **7542: Discrepancy in increasing CTME in continue runs (2005-03-03)**  
Change use of the CTME card so that it specifies the additional time to run the problem for continue runs. This is consistent with the all versions of MCNP.
- **7568: Recursive Monte Carlo bug (2005-03-08)**
- **7583: Incorrect calc. of tally segment surface area with identical surfaces (2005-03-15)**  
This bug goes back to at least MCNP4B and is caused by the fact that MCNP does not check for identical surfaces when it calculates areas for tally segments.
- **8256: Out-of-bounds ECH array (2005-05-03)**  
Corrected the allocation for the ECH array.
- **8456: Output statement overflows MESHTAL file record (2005-05-12)**  
Calculation of the maximum record length of the MESHTAL file did not take into account the extra line feed appended to the end of each record in a Windows file. Number of energy bins in the mesh was not included in the record length calculation.

- **8556: Code crashes on some user input file errors (2005-05-17)**  
Code will crash if there is a DE, DF, or FM card that is given an incorrect tally number, and there are no mesh tallies in the input file.
- **8659: FILE ALL command does not work with the interactive plotter (2005-05-23)**  
Problem with interactive geometry plotting subroutine with the variable which controls whether the plot is written to the metafile or not, JGF is always set to 0 (do not plot to the metafile) if the previous plot was written to the PLOT.PS file. A conditional was added so that JGF is not turned of if it has the value of 2 (FILES ALL mode).
- **8975: Bad format statement - ronge (2005-06-14)**  
Fixed a bad format statement in ronge.F90 - label 96, had an extraneous blank in the middle of a number
- **9440: PTY keyword of SSR card does not work (2005-07-14)**  
No coding was included to allow for single character data on the SSR card.
- **9582: Over indexing of SCF array in AXIS.F90 (2005-07-21)**  
Code tries to access elements of the scf array beyond its upper bound and causes the code to crash with an access violation error. The form of this do loop goes back to at least MCNP4B.

### Work in progress

The list below contains items that are known issues with MCNP 5 1.40. All of these items are works in progress.

- **6263: 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.
- **7101: Event log print error: npa= 0 from weight window split**
- **7353: Parallel calculations of VOV do not agree with sequential runs**
- **9438: 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.
- **9439: Source-in-repeated-structures problem**  
Defining source with optional forms '['] and ':' fails.
- **9443: Fully-specified fill plotter bug.**  
Incorrectly ordered fully-specified fill appears to be correct when plotted.
- **9641: Bad Interpolation in sampling bremsstrahlung photon energies**
- **9642: FIP Pinhole Image Tally With a TRCL on a Universe**  
Using an FIP pinhole image tally with a geometry that used a TRCL for a universe transformation produced incorrect results. When the same geometry uses individually transformed microbodies, all point detector tallies (F5, FIP, and FIR) give correct results.

- **9660: Fatal error for F8 tally with perturbation card**
- **9700: Incorrect f1:n tally segment result**  
Tally is posted in the wrong segment.
- **9852: Cannot allocate buffers in MPI for extremely large problems.**
- **10331: SDEF problem: EXT function of POS not working**  
If EXT is a function of position, then it appears that the EXT is not used. When the case is reversed, and POS is a function of EXT, then the source position is determined as expected.
- **10392: Fatal error for source distribution numbers more than 999**  
The MCNP manual says the source distribution numbers should not be greater than 999. Sometimes this causes problems as in the attached input file tb1001. The code crashes because not enough space is allocated.

## Compilers

MCNP 5 1.40 has improved support for newer Fortran 90 compilers. The compilers supported are listed below. The c compilers listed are those used in making the executables for distribution.

- **Fortran 90 compilers supported for Linux:**  
Absoft 9.0 (seq, mpi) ; Intel 9.0 (seq, mpi) ; Lahey 6.2c (seq, mpi, omp) Pathscale 2.1 (64-b Opteron) (seq, mpi) ; Portland Group 6.0 (seq, mpi, omp)
- **C compilers used for Linux executable:**  
Intel compiler executable: gcc version 3.2.3 20030502 (Red Hat Linux 3.2.3-53)  
Opteron executable: gcc version 3.4.4 20050721 (Red Hat 3.4.4-2)
- **Fortran 90 compilers supported for Mac OSX:**  
Absoft Pro 9.0 (seq, mpi) ; IBM XL 8.1 (seq, mpi)
- **C compilers used for Mac OSX executable:**  
gcc 3.3
- **Fortran 90 compilers supported for Windows 2000/XP:**  
Absoft 9.0 (seq) ; Compaq 6.6b (seq, mpi) ; Intel 9.0 (seq,mpi) ; Lahey 7.1 (seq)  
-MPI Parallel versions can be built using cygwin: For PCs, parallel versions of MCNP5 can be built from the cygwin command line with the Intel and Compaq fortran compilers. Add "mpi" to the config options or use the install script.
- **C compilers used for Windows 2000/XP executable:**  
gcc compiler on cygwin, version 3.4.4  
Microsoft Visual Studio .NET 2003 C/C++ compiler (with Compaq and Intel Fortran compilers)

## Additional Notes

### 1. Using the LETHARGY Command for Lethargy Normalization

Lethargy-normed plots of energy-dependent tallies with a log energy abscissa are made with the LETHARGY plotting command. This command cannot be used for cross-section plots. For this command to apply, "FREE e" must be active, "LOGLIN" or "LOGLOG" axes must be used, and the "NONORM" command must not be invoked.

The LETHARGY command cannot be used after a COPLOT command and can be disabled to return to energy bin-width tally normalization for a log energy abscissa by using RESET LETHARGY.

### 2. Using the mesh tally plotter

The mesh tally plotter operates in both the geometry plotter and the tally plotter modes. In the geometry plotter, to display the location of the mesh tally bins, use the command FMESH n, where n is the mesh tally number. Alternately, one can use the FMESH button of the interactive geometry plotter (located on the lower left of the screen) to select the tally to be plotted. The command FMESH off will turn off the mesh tally display.

To display the results of the mesh tally, MCNP invokes the geometry plotter. The default layout depends on the type of mesh tally. For rectangular meshes, the horizontal axis is in the direction of the dimension with the most number of bins, and the vertical axis is in the direction of the dimension with the second most number of bins. For cylindrical plots, the horizontal axis is along the axis of the cylinder and the vertical axis is along the theta=0 plane. The center of the plot in both cases is at the center of the mesh. Different views are obtained by using the MCNP geometry plotter commands. Exiting the mesh tally plotter will return the code to the tally plotter. Note: there are two ways to change the mesh that is plotted. One method is to use the FMESH button of the interactive plotter command panel. This will change the mesh tally but not the plot attributes (basis, extent, and origin). The second method is to enter the FMESH n command in the command box. This will reset the plot layout to the default for that particular mesh tally. The commands associated with the mesh tally plotter are:

- **FMESH** *n* Plot mesh tally *n*.
- **FMRELEERR** *n* Plot the relative errors of mesh tally *n*. If *n* is not provided, will plot the relative error for the current mesh
- **ZLEV** *n1 n2 n3 ...* Controls the scale of the mesh tally results.  
The parameters  $n_i$  can have the following values:
  - **log** sets the tally data scaling to logarithmic (default)
  - **lin** sets the tally data scaling to linear numeric value

If no values are given, sets the scale to the default for the particular color mode. If only one value is given, sets the lower limit of the plot. If two values are given, sets the lower and upper limits of the plot. If three or more values are given, sets the values of the

color gradients.

- **EBIN**  $n$  Plot energy bin  $n$  of the current mesh tally. The total energy bin is the last bin of the tally.

### 3. Using the neutron multiplicity treatment

For any fission reaction a number of neutrons,  $n$ , is emitted according to the value of  $\bar{\nu}$ . Depending on the type of problem (fixed source or KCODE) and on user input (TOTNU card), MCNP may use either prompt  $\bar{\nu}_p$  or total  $\bar{\nu}_t$ . For either case, the average number of neutrons per fission,  $\bar{\nu}$ , may be a tabulated function of energy or a polynomial function of energy.

If the fifth entry on the **PHYS:N** card is **zero** (default), then  $n$  is sampled between  $I$  (the largest integer less than  $\bar{\nu}$ ) and  $I + 1$  by:

- $n = I + 1$  if  $\xi \leq \bar{\nu} - I$
- $n = I$  if  $\xi > \bar{\nu} - I$ , where  $\xi$  is a random number.

If more microscopically correct fission neutron multiplicities are desired for fixed source problems, the fifth entry on the **PHYS:N** card can be used to select which set of Gaussian widths are used to sample the actual number of neutrons from fission that typically range from 0 to 7 or 8.

Fission neutron multiplicity distributions are known to be well reproduced by simple Gaussian distributions. The Gaussian widths given in the MCNP manual in Table 2.1 on pg 2-52 are used for fission multiplicity sampling in MCNP when the fifth entry on the **PHYS:N** card is **1**. Induced fission multiplicities for isotopes not listed in Table 2.1 use a Gaussian width that is linearly dependent on the mass number of the fissioning system. A number of factorial moments, as a function of  $\bar{\nu}$ , are reported in the output.

### 4. Using the stochastic geometry option

**Form:** **URAN**  $n1$   $dx1$   $dy1$   $dz1$   $n2$   $dx2$   $dy2$   $dz2$

- $n1$  = Universe number for applying stochastic transformation (only when used to fill a lattice element)
- $dx1$  = maximum translation in +/- x-direction
- $dy1$  = maximum translation in +/- y-direction
- $dz1$  = maximum translation in +/- z-direction
- $n2, dx2, dy2, dz2$  - optional second stochastic transformation universe and parameters

The **URAN** card provides a limited means of modeling stochastic geometry in MCNP for both fixed-source and eigenvalue problems. It is primarily intended for modeling the randomly located fuel kernels in high-temperature gas-cooled reactor (HTGR) geometries. This feature may have other possible applications, but users should proceed carefully and perform their own verification calculations to ensure that the feature adequately represents the physical problem they are modeling. Additionally, users should be extremely cautious in supplying information using the **URAN** card because MCNP has no means of checking whether the

supplied parameters properly represent the physical model being simulated.

#### 5. Using the new electron straggling algorithm

In the MCNP 5.1.40 release to RSICC, a new Fortran 90 module has been installed to deal with straggling data. Those parameters that are separate from the individual straggling events are still precomputed, but each electron transport step can now sample its energy loss separately from adjacent steps, and specifically for its current energy and planned step length. Using this approach, we largely eliminate the linear interpolations and energy misalignments of the earlier algorithms and obviate the need for a choice of energy group. At the time of the MCNP 5.1.40 release, the new straggling logic is included in the code, but is still being tested. Preliminary results indicate that a more accurate and stable estimate of the straggling is obtained, and a variety of unphysical artifacts are eliminated.

The new logic is selected by setting the 18th entry of the DBCN card to 2, for example with the card "**DBCN 17J 2**".

#### **Installation instructions**

Un-installation of previous version of MCNP is recommended. Installation of the latest release of MCNP, RSICC version 5.1.40, is the same as described in the PDF file 'MCNP5\_Install\_Guide.pdf'. No patch file will be distributed to update the previous version of MCNP.

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