

LA-UR-10-07031

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Title: MCNPX 2.7.D Extensions

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Intended for: <http://mcnpx.lanl.gov>



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by

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October 18, 2010

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MCNPX 2.7.D Extensions

ABSTRACT

MCNPX is a Fortran90 Monte Carlo radiation transport computer code that transports nearly all particles at nearly all energies for nearly all applications. The new capabilities of the latest version, MCNPX 2.7.D, beyond those in MCNPX 2.6.0, are described.

1 INTRODUCTION

MCNPX (MCNP eXtended) is a Fortran90 (F90) Monte Carlo radiation transport computer code that transports nearly all particles at nearly all energies. It is a superset of MCNP4C3 and has many capabilities beyond MCNP4C3. MCNPX is a production computer code that models the interaction of radiation with matter. Its quality is highly regarded and cash awards (described in Section 1.4) are offered for bugs.

1.1 SUMMARY OF NEW MCNPX FEATURES

The new capabilities and enhancements of MCNPX 2.7.D beyond MCNPX 2.6.0 are listed below. (Where applicable, the initials of the principal developers are shown in parentheses.¹) Note that the arithmetic MPLOT capability is developmental. It is not backed by the MCNPX cash awards quality assurance program and must be used cautiously. However, this capability is considered of such significance that it is included. Recall also that as of version 2.6.0 total v (not prompt v) is the default for fission neutrons. The new MCNPX 2.7.D capabilities include the following:

- Tally tagging (GWM)
- CEM 3.02 upgrade (MRJ/SGM)
- Plot appearance upgrades (JWD/LSW)
- Embedded sources (JSH)
- Stopping power energy table control (GWM)
- Cyclic time bins (GWM)
- Focused beam sources (JWD/JSE/LSW)
- PTRAC coincidence option (WCS/MRJ)
- LLNL photofission multiplicity (JMV/GWM)
- Arithmetic MCPLLOT options (JWD/LSW)
- Receiver-operator characterization (ROC) tally option (GWM)
- Pulse-height light tally: triple and quadruple coincidences (GWM)
- Time-dependent F8 tallies using the pulse-height light option (GWM)

¹ Joe W. Durkee (JWD, LANL, D-5), Jay S. Elson (JSE, LANL, D-5), Michael L. Fensin (MLF, LANL, D-5), John S. Hendricks (JSH, TechSource); Michael R. James (MRJ, LANL, D-5), Russell C. Johns (RCJ, LANL, D-5), Gregg W. McKinney (GWM, LANL, D-5), Stepan G. Mashnik (SGM, LANL, X-3-MCC), Jerome M. Verbeke (JMV, LLNL), Laurie S. Waters (LSW, LANL, D-5)

- Extensions and enhancements
- Corrections

1.2 AVAILABILITY

The latest general-release version is MCNPX 2.6.0, which is available from the Radiation Safety Information Computational Center (RSICC)¹.

For approved users, beta test program versions may be downloaded from the MCNPX website.² Approximately 2000 MCNPX beta test users are an essential part of the MCNPX software quality assurance program. In general, to become a new beta test user usually requires being an MCNPX sponsor, collaborator, or participant in an MCNPX workshop training course. For more information, contact us at the following address: mcnp@lanl.gov.

MCNPX is U.S. export controlled. Generally, MCNPX is easy to obtain for legitimate purposes, but restrictions protect the code, data, and documentation once it is acquired.

1.3 DOCUMENTATION

Restricted Documentation:

Complete MCNPX documentation is available in the “MCNPX™ User’s Manual Version 2.6.0,”³ which comes with MCNPX from RSICC and is available to MCNPX beta testers from the MCNPX website.⁴

Unrestricted Documentation:

Documentation of MCNPX features in MCNPX 2.5.0—that is, all MCNPX features beyond MCNPX 2.3.0 and MCNP4C—is provided in “MCNPX Extensions, Version 2.5.0.”⁵ Similarly, features beyond MCNPX 2.5.0 that appear in MCNPX 2.6.0, are described in “MCNPX 2.6.0 Extensions.”⁶

MCNPX capabilities developed since MCNPX 2.6.0 are documented in this report.

All of the extended MCNPX capabilities are summarized in the one-page MCNPX features list.⁷

1.4 CASH AWARDS QUALITY ASSURANCE PROGRAM

We are so confident in the quality of MCNPX that MCNPX Development Team offers cash awards to the first person who finds any bug in the code. They will pay \$20 to the first person finding anything that does not meet or exceed the capabilities of MCNPX 2.3.0 and MCNP4C3.

¹ <http://rsicc.ornl.gov/>

² <http://mcnp.lanl.gov/beta>

³ Denise B. Pelowitz, ed., “MCNPX User’s Manual, Version 2.6.0,” Los Alamos National Laboratory report, LA-CP-07-1473 (April 2008), http://mcnp.lanl.gov/docs/MCNPX_2.6.0_Manual.pdf/.

⁴ <http://mcnp.lanl.gov/>

⁵ <http://mcnp.lanl.gov/opendocs/reports/Interface.pdf/>

⁶ <http://mcnp.lanl.gov/opendocs/versions/v260/v260.pdf>

⁷ <http://mcnp.lanl.gov/opendocs/misc/FeaturesList.pdf/>

European users will be awarded €20. They also will pay a brand new \$2 bill for any error in MCNPX that has been inherited from its constituent codes.¹ A list of all winners since June 2001 can be found on the MCNPX website.²

2 DESCRIPTION OF NEW MCNPX FEATURES

Note that the criticality source convergence acceleration capability is developmental. This capability is not backed by the MCNPX cash awards program and must be used cautiously.

The principal new capabilities of MCNPX beyond MCNPX 2.6.0 described in detail in this section are

- Tally tagging
- CEM 3.02 upgrade
- Plot appearance upgrades
- Embedded sources
- Stopping power energy table control
- Cyclic time bins
- Focused beam sources
- PTRAC coincidence option
- LLNL photofission multiplicity
- Arithmetic MCNPLOT options
- Receiver-operator characterization (ROC) tally option
- Pulse-height light tally: triple and quadruple coincidences
- Time-dependent F8 tallies using pulse-height light option

2.1 TALLY TAGGING

Tally tagging, a new feature, provides the ability to separate a tally into components based on how and where the scoring particle was produced. This feature is available for both standard and detector tallies; however, it is only implemented for neutron, photon, and electron tallies.

2.1.1 User Interface

Tally tagging is specified by using the new keyword, TAG, with its associated parameter, a , on the FT n tally special treatment card, which is associated with a standard F n tally. The format is

```
FT $n$     TAG     $a$ 
```

where n is the neutron or photon tally number, and a specifies how scatter is to be treated (i.e., whether the creation tag on a particle should be retained or a separate scatter tag be invoked):

¹ Cash Award Fine Print: This offer is subject to cancellation or modification without notice. A bug is defined as an error we choose to correct in the source code. We make awards even for the most trivial or insignificant of problems, but not for proposed code enhancements or proposed extended capabilities. Awards are given only to the first MCNPX user reporting a problem. MCNPX development team members are ineligible. Reported problems must be reproducible, and awards are paid when the correction is integrated into a forthcoming MCNPX version. We endeavor to make MCNPX the most error-free and robust Monte Carlo radiation-transport code possible, and we back this code with a cash award.

² <http://mcnp.lanl.gov/opendocs/misc/Cashbugs.pdf/>.

- a=1 indicates that all collided particles will lose their tag and that bremsstrahlung and annihilation photons will be included in the bin of collided particles;
- a=2 indicates that all collided particles will lose their tag, but that bremsstrahlung and annihilation photons will be given special tags that allow them to be segregated; and
- a=3 indicates that all collided particles will retain their production tag.

Binning specifications for the tagged tally must be provided on the FU special tally card. Each bin_i (described below) requests three distinct pieces of tagging information:

- 1) a cell of interest where particles are produced;
- 2) a target nuclide from which the particle is emitted; and
- 3) a reaction or, in the case of spallation, a residual nuclide of interest.

The format on the FU card when used in association with the tagging treatment is

```
FUn  bin1 bin2 ... binN [NT]
```

where each tagging bin_i has the form CCCCCZZAAA.RRRRR. A user cell number is designated by CCCC (leading zeros are not required); ZZAAA represents a five-digit isotope identifier for a target nuclide, where ZZ represents the atomic number and AAA represents the atomic mass number and RRRRR specifies a reaction identifier for library interactions or a residual nuclide ZZAAA identifier for high-energy model interactions. Special cases for the CCCCCZZAAA.RRRRR FU card entries are provided in Section 2.2.2. Note that the ZZ atomic number specification is limited to two characters; therefore nuclides with $Z > 99$ cannot be tagged. By default, a total over all specified bins is provided automatically for the FU special tally. To suppress the generation of a total, add the "NT" parameter after the last specified bin.

2.1.2 Usage and Special Cases

If cell tagging is not desired, the CCCCC portion of the tag should be omitted or, alternatively, set to "00000". In either case, tally contributions will be accumulated for all cells for that FU bin, provided the ZZAAA.RRRRR portion of the tag is satisfied. In the case of particle production from electrons, which are material based (not nuclide specific), the CCCCC input should be used to identify the cell and the ZZAAA input should be set to "00000". The suffix RRRRR refers to a standard ENDF reaction number for library interactions (e.g., "00102" stipulates $[n,\gamma]$) or, in the case of high-energy model interactions, RRRRR refers to a residual nuclide ZZAAA identifier (e.g., "06012" for ^{12}C). Additional library-related reactions numbers can be found in Appendix G of the MCNPX User's Manual.

In general, a zero input for any portion of the tag results in the sum of all contributions related to the entry. For example, the tag "0000092000.00000" will collect all tally contributions where any isotope of uranium ($z=92$) had produced the particle making the tally. However, the tag "0000000000.00000" is reserved for elastic-scattered particles. Note that each tally contribution is made only to the first FU bin that satisfies the tag description (i.e., those that have not already been tallied). If no appropriate FU bin is found, the tally contribution is not made; however a special "everything else" bin_i (i.e., "1e10") can be specified to collect any portion of the tally that falls into no other bin. When the "everything else" bin is used, then the user is assured that

the “user-bin total” bin will reproduce the original tally as if the `F1:n TAG` option has not been used.

Special designations for `CCCCCZZAAA`:

<code>-0000000001</code>	or	<code>-1</code>	source particle tag for all cells
<code>-CCCCC00001</code>			source (i.e., uncollided) particle tag for cell <code>CCCCC</code>
<code>0000000000</code>	or	<code>0</code>	elastic-scattered particle tag
<code>10000000000</code>	or	<code>1e10</code>	everything else tag

Photon tally special designations for `ZZAAA.RRRRR`:

<code>00000.00001</code>	bremsstrahlung from electrons
<code>ZZ000.00003</code>	fluorescence from nuclide <code>ZZ</code>
<code>00000.00003</code>	K x-rays from electrons
<code>00000.00004</code>	annihilation photons from e^-
<code>ZZ000.00005</code>	Compton photons from nuclide <code>ZZ</code>
<code>ZZAAA.00006</code>	muonic x-rays from nuclide <code>ZZAAA</code>

Electron tally special designations for `ZZAAA.RRRRR`:

<code>ZZ000.00001</code>	photoelectric from nuclide <code>ZZ</code>
<code>ZZ000.00003</code>	Compton recoil from nuclide <code>ZZ</code>
<code>ZZ000.00004</code>	pair production from nuclide <code>ZZ</code>
<code>ZZ000.00005</code>	Auger electron from nuclide <code>ZZ</code>
<code>00000.00005</code>	Auger electron from electrons
<code>00000.00006</code>	knock-on electrons

Neutron and photon tally special designations for `ZZAAA.RRRRR`:

<code>ZZAAA.99999</code>	delayed particles from fission of <code>ZZAAA</code>
--------------------------	--

2.1.3 Examples

Example 1:

```
F1:N 10
FT1 TAG 1
FU1 0000092235.00016 0000092235.0000 1e10
```

If an `[n,2n]` neutron that is produced from an interaction with ^{235}U contributes to the `F1` tally, then its contribution will be included only in the first `FU` bin even though its tag also will satisfy the criteria for the 2nd `FU` bin. Thus, the order of the `FU` bin tags is important for segregating the tally. Note in this example that neutrons produced by some other reaction with ^{235}U will be placed in the 2nd `FU` bin and neutrons produced by reactions with other target nuclides will be placed in the last (“everything else”) bin. The sum of these three bins should preserve the value of the original `F1:N` tally.

Example 2:

```

F1:P  1
FT1  TAG  1
FU1  0.0  01001.00102  01001.00000
        26056.00102  26056.00051  26056.00052
        26056.24052  26056.26053  26056.26054  26056.26055
        26056.00000

```

In this case, all elastic-scattered photons (i.e., coherent) will be put into the FU “0.0” bin. All capture gammas from ^1H will be put into the 01001.00102 bin; all remaining gammas from ^1H interactions will be put into the 01001.00000 bin. All capture gammas from ^{56}Fe will go into the 26056.00102 bin; all [n,n'] 1st level gammas will go into the 26056.00051 bin; all [n,n'] 2nd level gammas will go into the 26056.00052 bin; all deexcitation gammas from the spallation of ^{56}Fe into ^{52}Cr will go into the 26056.24052 bin; etc. All remaining gammas produced from ^{56}Fe interactions will go into the 26056.00000 bin.

Example 3:

```

F5:P  0 0 0 1
FT5  TAG  3
FU5  -1.0  0000106012.00005  0000106012.00000
        0000026056.00102  0000026056.00000
        0000000000.00051
        1000000000.00000

```

In this case, all collided photons will retain their original creation tag. All source photons will go into the -1.0 bin. All Compton photons from ^{12}C in cell 1 will be put into the 2nd bin; all remaining photons produced from interactions with ^{12}C in cell 1 will go into the 3rd bin. All capture gammas from ^{56}Fe will go into the 4th bin; all remaining photons/gammas produced from interactions with ^{56}Fe will go into the 5th bin. All [n,n'] 1st level gammas will be put into the 6th bin, and all remaining photons/gammas that were not included in any of the previous bins will be placed in the last bin.

2.2 CEM 3.02 UPGRADE^{1,2}

In versions 03.02 of CEM and LAQGSM, the Fermi breakup model is used at all stages of a reaction for an excited nucleus with atomic mass $A < 13$. Previously, in versions 03.01 of these codes, the Fermi breakup model was used to calculate the disintegration of light nuclei but was not used at the preequilibrium, evaporation, and fission stages for an excited nucleus or a fission fragment with $A < 13$.

¹ S. G. Mashnik, R. E. Prael, and K. K. Gudima, "Implementation of CEM03.01 into MCNP6 and its Verification and Validation Running through MCNP6. CEM03.02 Upgrade," research note X-3-RN(U)-07-03, Los Alamos National Laboratory (2007).

² S. G. Mashnik, K. K. Gudima, R. E. Prael, A. J. Sierk, M. I. Baznat, and N. V. Mokhov, "CEM03.03 and LAQGSM03.03 Event Generators for the MCNP6, MCNPX, and MARS15 Transport Codes," invited lectures presented at the Joint ICTP-IAEA Advanced Workshop on Model Codes for Spallation Reactions, February 4–8, 2008, ICTP, Trieste, Italy, Los Alamos National Laboratory report LA-UR-08-2931 (2008); E-print: arXiv:0805.0751v2 [nucl-th]; IAEA Report INDC(NDS)-0530, Vienna, Austria, August 2008, p. 53.

Also, the computer routines that describe the Fermi breakup model, written by the original authors in Russia twenty years ago, historically have had some occasional odd behavior. These problems have been corrected in version 03.02. First, no longer do these routines allow the rare production of some light unstable fragments like ^5He , ^5Li , ^8Be , and ^9B as a result the breakup of some light excited nuclei. Also no longer permitted is the very rare production of “neutron stars” or “proton stars,” that is, the production of residual nuclei produced via Fermi breakup that consist of only neutrons or only protons. Code crashes caused by an occasional division by zero within the Fermi breakup routines have been eliminated as have several other coding bugs.

CEM 3.02 was integrated into MCNP6 and MCNPX by H. Grady Hughes and Richard E. Prael. The 03.02 versions of CEM and LAQGSM more correctly describe nuclear reactions on intermediate and light nuclei and the production of fragments heavier than ^4He from heavy targets than did their predecessors. Additionally, these new versions produce very few unstable unphysical final products and are free of the corrected bugs.

The file mollinix.tbl is now in the MCNPX data files and is required for CEM 03.02.

A graphical comparison of Bertini, CEM 03.01, and CEM 03.02 appears in Figures 1 and 2. The plots are results of neutron flux near a proposed tungsten target at the LANL LANSCE facility. The driver for the plotted flux was an 800-MeV proton beam. Overall, the energy spectra show very good agreement between the CEM versions, but the comparison is not as good with Bertini.

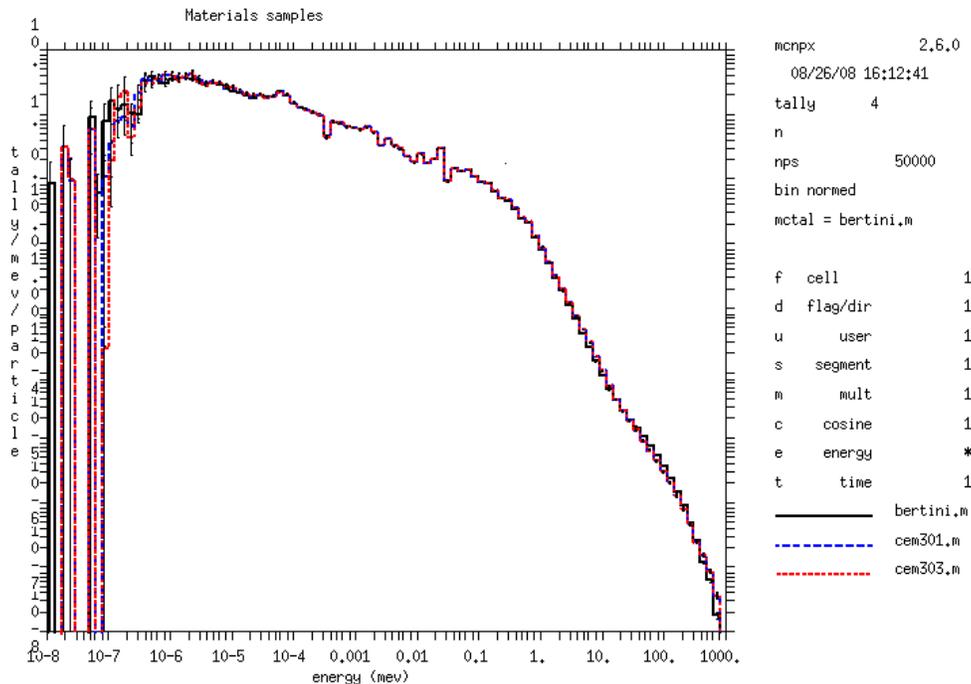


Figure 1. Neutron flux generated by an 800-MeV proton beam in LANSCE material samples. (Note that CEM 03.02 is mislabeled as “cem303” in the plot.)

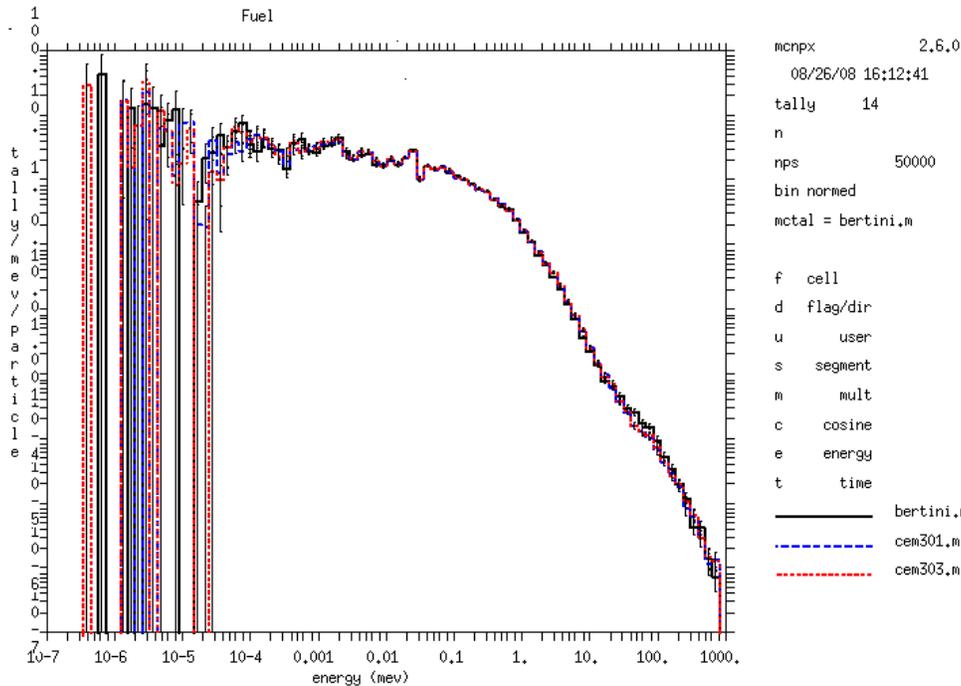


Figure 2. Neutron flux generated by an 800-MeV proton beam in LANSCE fuel sample. (Note that CEM 03.02 is mislabeled as “cem303” in the plot.)

2.3 MC PLOT GRAPHICS AND “HELP” COMMAND UPGRADES ¹

MC PLOT has been upgraded, providing improved appearance of graphics and an enhanced help package. MC PLOT plots table-range cross-section data, tallies, and other quantities such as convergence criteria and criticality parameters. Among these improvements are the following:

- Significantly improved help package with alphabetized commands and the capability of retrieving short descriptions of each command with its options.
- Capitalized fonts and capitalization of code-supplied titles and quantities. Among other things, “mev” is now “MeV.”
- Horizontally displayed y-axis labels.
- Enable 70-character plot titles.
- Increase the maximum dynamic range for plotting of tally and other data from 17 to 35 orders of magnitude. This allows time phenomena from nanoseconds to years can be placed on a log plot.
- Allow log10 axes for contour plots.

2.3.1 Graphics Upgrades

Among the graphical improvements are the following:

¹ J. W. Durkee, et al., "MCNPX Graphics and Arithmetic Tally Upgrades," International Conference on Mathematics, Computational Methods, & Reactor Physics (M&C 2009), Saratoga Springs, New York, May 3-7, 2009.

Improved readability and flexibility of axis values: Ordinate values are now displayed horizontally and the default print density of the numbering on each axis has been adjusted to eliminate overcrowding. This default density of the axes tick values can be overridden by the user using the *nsteps* parameter on the *XLIMS* and/or *YLIMS* command. For logarithmic plots, larger tick marks now signify major decades while smaller marks indicate values between decades. The number of decades that can be displayed on a logarithmic plot has been increased from 17 to 35. This increase allows time phenomena from nanoseconds to years to be placed on a logarithmic plot. Also, use of the “e” format to represent scientific notation decreases the tick label length and consequently enhances readability.

Axes and legend labels: For energy plots, the default units now read “MeV” instead of “mev” and the first letter of each word in default axis labels is now capitalized. Character limits for legend labels have been increased: the graphical line-pattern identifiers have been shortened and the text region increased, allowing up to 23 characters to be displayed in the legend label. Main titles up to 70 characters long are now permitted for both screen and PDF plots.

Information and legend blocks: The first letter of the left-aligned tally bin type is now capitalized and the *probid* is included in the information block to explicitly indicate the date and time stamp of the *RUNTPE* or *MCTAL* file instead of the build date of the executable.

Figure 3 illustrates several plot upgrades, including (1) longer titles, (2) legend problem identification (*probid*), (3) alignment of legend tally type labels, (4) increased length of legend curve identifiers, (5) capitalized letters for axes and legend labels, (6) horizontal display of ordinate numbers, and (7) wider major ticks for logarithmic axes.

Figure 4 illustrates (1) 35-decade logarithmic-axis plot capability, (2) wider ticks at major logarithmic-axis decades, (3) automatic refinement of the number of minor ticks, (4) automatic refinement of the number density on logarithmic axes.

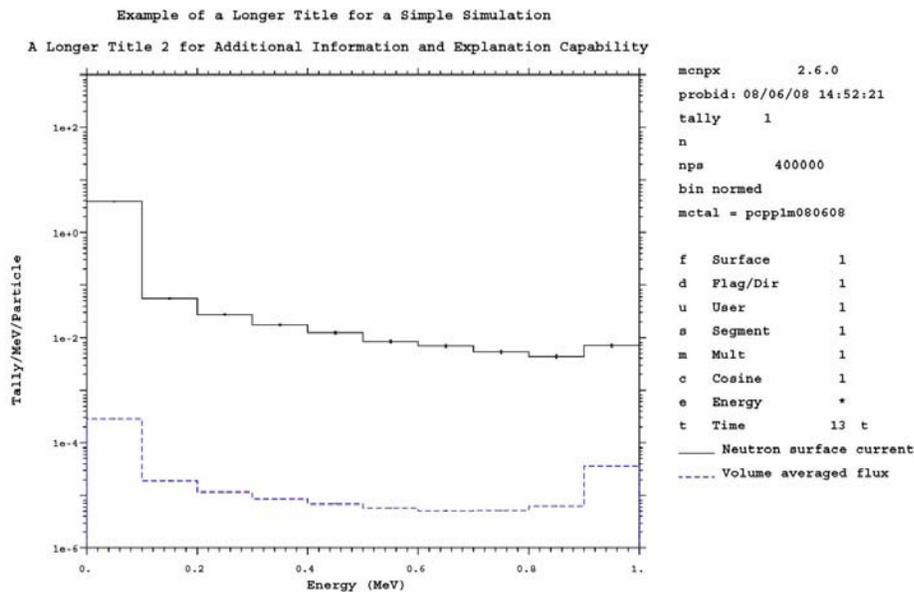


Figure 3. Upgraded MCPLLOT 2-D tally graphics.

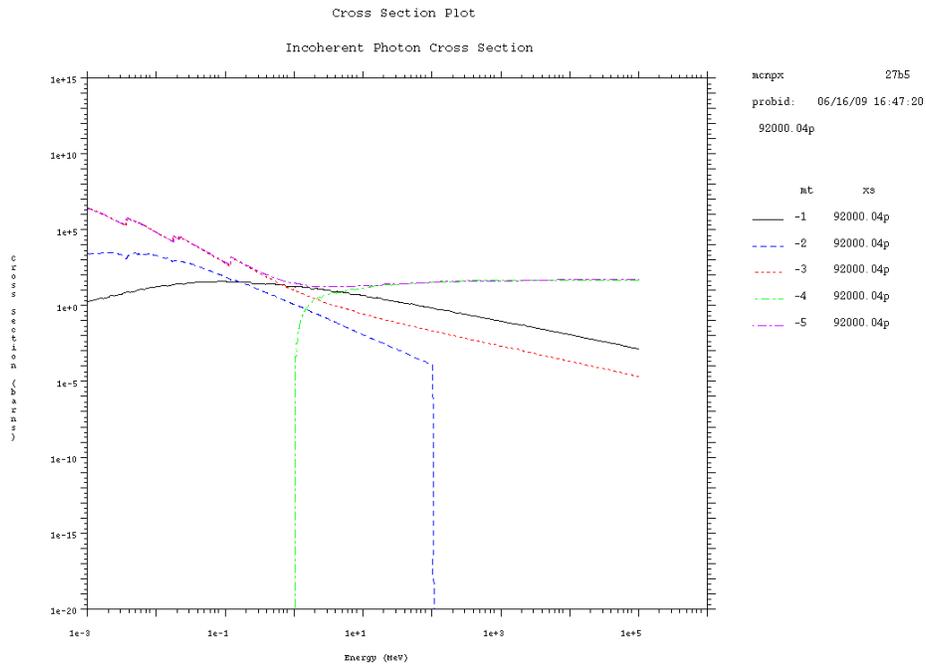


Figure 4. Upgraded MCNPLOT cross-section plot graphics.

Contour plots: Contour plots may now be created using logarithmic axes. In addition, contour-plot legend information now ranges from low to high as one moves up the page.

Figure 5 illustrates (1) the use of logarithmic-axis plotting for contour plots and (2) legend decade identifiers ranging from low to high, moving up the page.

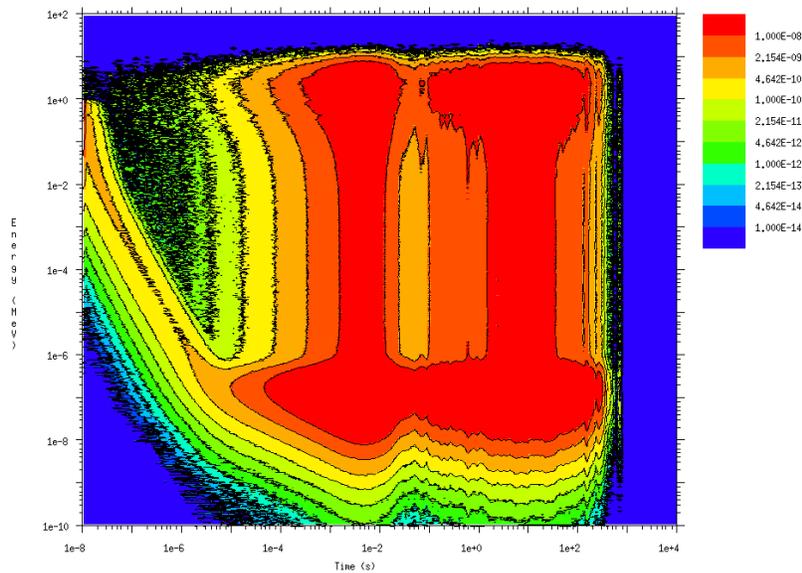


Figure 5. MCNPLOT log-scale contour plot.

Example:

The contour plot in Figure 5 represents the energy versus time relationship of the neutron flux in a 100-cm-radius sphere of water that includes a small amount of ^{235}U . The water sphere encompasses a 1-MeV isotropic point source of neutrons. The contour plot was created using the following input file, which includes an embedded call to the MCPLLOT tally plotter:

```
Test problem for 2D mcplot log10-axis contour plots
1      1 -1.0 -100  imp:n=1 $ Water sphere with U-235
9000  0          100  imp:n=0 $ Outside void

100  so  100.0

m1      1001.66c 2  8016.66c 1  92235.66c 0.001  $ H2O+U-235 (1g/cc)
mt1     lwtr.64t
c
mode    p n
phys:n  3j -101      $dn by models
phys:p  5j -101      $dg by models, mg+lines
cut:n   j j 0        $ Force analog capture
sdef    par=n erg=1  $ 1-MeV isotropic point source
nps     le6
prdmp   j j 1 j -1  $Third entry 1 writes code name, etc.
mplot   tal 4 free et loglog con 1e-14 1e-8 log xtitle "Time (s)" &
        ylimits 1e-10 100 factor x 1e-8 xlims 1e-8 1e4 freq 200000
c
fc4     f4 volume-integrated flux
f4:n    1
e4      1.0e-10 999log 1000
t4      1.0 199log 1e12
```

Alternatively, the contour plot can be generated from the RUNTPE or MCTAL files after the run has completed.

2.3.2 “HELP” Command Upgrade

The MCNPX MCPLLOT “HELP” command has been upgraded to improve its functionality. With the exception of the arithmetic tally commands (discussed in Section 2.10), the four-column listing of HELP commands is now alphabetized. In addition, tips appear at the bottom of the four-column list of HELP commands to indicate how to

- 1) invoke a listing of all HELP commands with an explanation of their function and use syntax (“HELP ALL”),
- 2) provide a listing of function and syntax for a single HELP command (“HELP <command>”),
- 3) request an overview of the MCPLLOT capability (“OVERVIEW”), and
- 4) summarize input and execution-line options (“EXECUTE”).

To further aid the user, some commands are now cross-referenced to guide the user toward related commands that may be of interest.

Example 1: After invoking the MCPLLOT utility, if you enter the command “HELP”, you will receive the following response:

```
mcplot>
help
Available commands:
      bar          loglin      spline          3d
      below        loglog      status          +
      contour      mt          subtitle        -
      coplot       noerrbar   tally           *
      dump         nonorm     term            /
      end          options    tfc            (
      factor       par         thick           )
      file         pause      thin           =
      fixed        pert         title          patalcmd
      free         plinear   view           rzmctal
      freq         plot       wmctal        wzmctal
      help         printal   xlims          exp
      hist         printpts  xs             ln
      iptal        reset      xtitle        log10
      kcode        return    ylims          sqrt
      label        rmctal   ytitle        ^
      legend       runtpe   ztitle        infinity
      linlin       scales   &             font
      linlog       set         ?

Type "help all" for a verbose list of all help commands
"help <command>" to list a specific help command,
"help overview" for an overview of MCPLLOT,
or "help execute" for MCPLLOT input & execution-line
options.
mcplot>
```

Example 2: After invoking the MCPLLOT utility, if you enter the command “HELP legend,” you will receive the following response:

```
mcplot>
help legend
  legend > Syntax: legend [x y]
          Include or omit the legend according to the values of
          optional parameters x and y.
          If no x and no y, put the legend in its
          normal place. (DEFAULT)
          If x=0 and no y, omit the legend.
          If both x and y are defined, for 2-D plots only,
          Put most of the legend in its usual place,
          but put the part that labels the plot lines at
          location x,y.
          Units for x and y are the units used for
          the x and y axes.
          The maximum legend curve label length is
          23 characters.
          See "label".

mcplot>
```

2.4 EMBEDDED SOURCES

MCNPX now allows source distributions to be embedded within each other to describe accelerator beam timing from micro- to macro-pulses as well as other sources that vary regularly.

2.4.1 User Interface

The format to specify an embedded source is

```
SDEF   TME = ( D11 < D12 < D13 )
```

or, for distributions of distributions, the following form may be used:

```
SDEF   TME = D41
SI41   S  51  ( D11 < D12 < D13 ) 52
```

In both cases, distributions 11, 12, 13 are all for the same variable, time. Distribution 11 covers a small time range that is repeated as often as needed to exactly fill the larger time range of distribution 12. Similarly, distribution 12 is repeated as often as needed to exactly fill the even larger time range of distribution 13.

Note that the parentheses are optional and that the designator “D” on the SI card with “S” option is also optional. Thus

```
SDEF   TME = ( D11 < D12 < D13 )   and
SDEF   TME =  D11 < D12 < D13     are equivalent.
```

Also,

```
SI41   S  51  ( D11 < D12 < D13 ) 52   ,
SI41   S  51   D11 < D12 < D13   52   ,
SI41   S  51  (  11 <  12 <  13 ) 52   , and
SI41   S  51   11 <  12 <  13   52   are all equivalent.
```

The embedded distributions must start at zero or a fatal error message is issued. For (D11<D12<D13) the lowest value on the SI11 and SI12 cards must be zero. The embedding distribution, D13, can have any range.

The embedded distributions should fit within each other (nearly) exactly. If they do not there is a fatal error message, “embedded distribution *nn* has improper range” and the distribution will spill into the next bin and have a strange normalization for values in its last bin.

Only continuous source distributions such as ERG, TME, X, Y, Z, DIR, RAD and EXT may use embedded distributions.

2.4.2 Examples

Example 1:

```
sdef   tme= d11<d12<d13
si11  0 1 2
sp11  0 1 0
```

```

si12 0 100 150
sp12 0 1 0
si13 -150 900
sp13 0 1
    
```

Figure 6 shows the MCNPLOT plot (MCNPX Z option) of the tally of this source in a vacuum during the time regime ranging from -200 to 1000 shakes. The seven repetitions of distribution 12 (which is described in SI12 as ranging from 0 to 150 shakes) are clearly seen embedded within distribution 13 (which describes the time period from -150 to 900 shakes.)

Figure 7 shows the MCNPLOT plot from -5 to 25 shakes. The 1st 13 of a total 50 repetitions of distribution 11 (which are each two shakes in duration) are seen in the first part of the 2nd repetition of distribution 12.

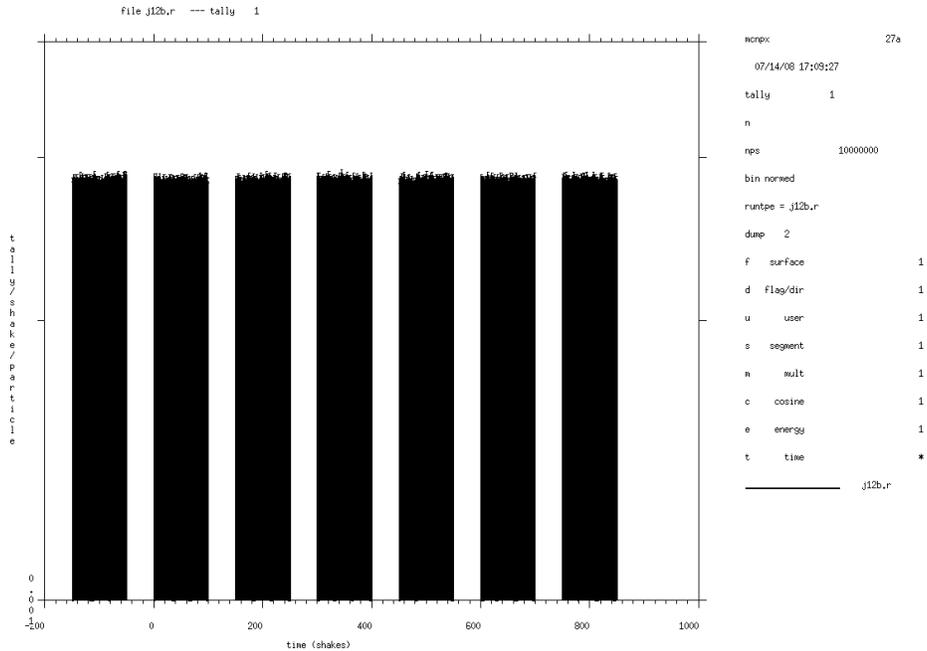


Figure 6. MCNPLOT plot of tally from -200 to 1000 shakes shows embedded pulses defined by distribution 12.

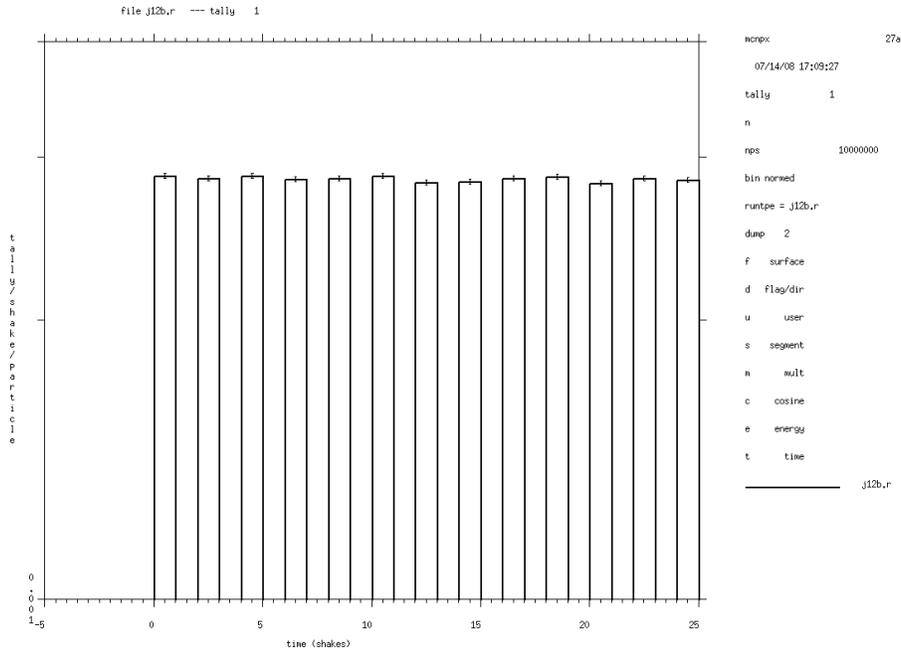


Figure 7. MCNPLOT plot of tally from -5 to 25 shakes, displaying embedded pulses defined by distribution 11.

Example 2 (embedding a distribution of distributions):

```
sdef erg d21 cel=d11 tme=d41
si41 S 52<51 (D31<32<d33) 61
sp41 .1 .8 .1
si51 A -26 -16
sp51 0 1
si52 H 0 1 2
sp52 0 1 0
si61 A 32 40
sp61 1 0
si31 0 1 2
sp31 0 1 0
si32 0 16
sp32 -41 8 8
si33 -16 32
sp33 0 1
```

This more complex example illustrates how embedded distributions can reside within distributions of distributions (D41), and can use built-in functions (D32 uses a Gaussian centered at $t=8$ with $FWHM=8$) and interpolated distributions (D51 and D61 use the SI A option). Distribution D52 is embedded in distribution D51; distribution D31 is embedded in distribution D32, which is embedded in distribution D33. The tally plot is in Figure 8.

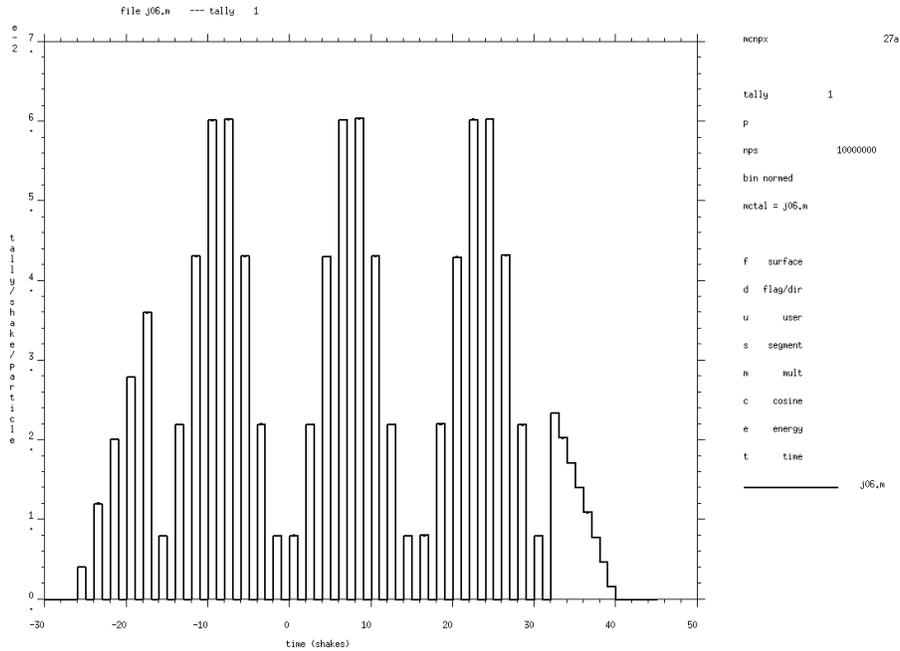


Figure 8. MCPLLOT plot of tally from -30 to 50 shakes.

2.5 STOPPING POWER ENERGY TABLE CONTROL

An 11th entry on the `PHYS:<pl>` card, where `<pl>` is any charged particle type, now controls the stopping power table energy spacing. This 11th entry is the parameter `efac`. Entries 6 through 10 on the `PHYS:<pl>` card are currently not used; therefore, when adding a value for `efac`, a “5J” entry must precede it. When `efac` is specified, the energy fraction (`efac`) for stopping power tables is the following:

$$E_{n-1} = E_n * efac$$

This applies to charged particles only. The value of `efac` is limited to $0.8 \leq efac \leq 0.99$. A larger `efac` produces more points in the stopping power tables. Default is `efac` = 0.917.

2.6 CYCLIC TIME BINS

An enhancement of the tally time-bin card, `T`, allows cyclic time bins to be automatically created and applied. The entries needed to create cyclic time bins are specified on the `T` card using the following keyword form:

`Tn` KEYWORD=*value*(s)

where the allowed keywords are

- CBEG reference starting time in shakes (sh) (default=0)
- CFRQ frequency of cycling in 1/sh or 1/time width
- COFI dead time interval in shakes
- CONI alive time interval in shakes

CSUB number of subdivisions to use within alive time (default=1)
 CEND reference ending time in shakes (optional)

If CEND is specified, all cyclic time bins are generated for the first cycle and these are repeated out to the CEND time. This allows one to easily determine the rise and fall in these cyclic bins over time. Basically this reverts to standard time-bin treatment, except that the bins are automatically produced.

Example:

```
T1    CBEG=0.0    CFRQ=1000e-8    COFI=0.000005e-8    CONI=0.0005e8    CSUB=5
```

This example specifies a reference starting time of 0 sh with a frequency of 1000 Hz ($1e-5 \text{ sh}^{-1}$). The dead time of 5 μs (COFI) results in a time bin from 0–500 sh that includes missed tally scores during the dead time. The alive time of 0.5 ms (CONI), with the specified five subdivisions (CSUB), results in five time bins equally spaced from 500–50500 sh. A final time bin from 50500–100000 sh will be provided for tally scores made after the alive time. Note that using the “e8” and “e-8” form shown here makes it easy to couch the entries in seconds and Hertz rather than using the native unit of shakes.

2.7 FOCUSED BEAM SOURCE OPTION¹

Using accelerator beam parameters, MCNPX can now simulate a charged-particle beam that has been produced by an accelerator and focused using a magnet-lens system. The code does not transport the beam through the magnetic and electric accelerator fields, but can apply the emittance factors of the beam leaving a focusing system. The beam is assumed to be transported in a field-free drift region. This capability is useful not only for accelerator beams, but can be applied to scenarios where a planar, circular, or elliptical source of particles must be focused toward some point.

As shown in Figure 9, our beam option consists of a particle beam with a circular (or, more generally, an oval) cross section emitted at $z=0$ for a beam envelope that is parallel to the direction of longitudinal transport, termed to be the z -axis. Particles that have been produced by an accelerator and focused using a magnet-lens system are started at the aperture. The beam is transported through drift space. The goal is to transport a beam that has been focused for a minimum spot size at a given distance (L) under the constraints of aperture size and emittance. In general, the waist of the beam envelope (i.e., the location of minimum radius and zero envelope slope) does not coincide with x_L , the beam half-width at distance L . Instead the waist is located at z_w , which is less than L .

2.7.1 User Interface

To describe a focused charged-particle beam source, two new keywords have been added to the SDEF card. The keyword BEM is used to specify beam emittance parameters while BAP specifies beam aperture parameters. More specifically,

¹ J. W. Durkee, et al., "An MCNPX Accelerator Beam Source," Los Alamos National Laboratory report LA-UR-09-03509 (2009), also *Progress in Nuclear Energy* **52**, pp. 544–554 (2010)

$$\text{BEM} = \text{exn} \text{eyn} \text{bml}$$

where

exn is the normalized beam emittance parameter, ε_{nx} , for phase-plane coordinates x, x' (π -cm-radians),

eyn is the normalized beam emittance parameter, ε_{ny} , for phase-plane coordinates y, y' (π -cm-radians), and

bml is the distance from the aperture to the spot, L (cm); and

$$\text{BAP} = \text{ba1} \text{ba2} \text{U}$$

where

ba1 is the beam aperture half-width in the x transverse direction, x_0 (cm),

ba2 is the beam aperture half-width in the y transverse direction, y_0 (cm), and

U is unused, but must be set to any arbitrary value.

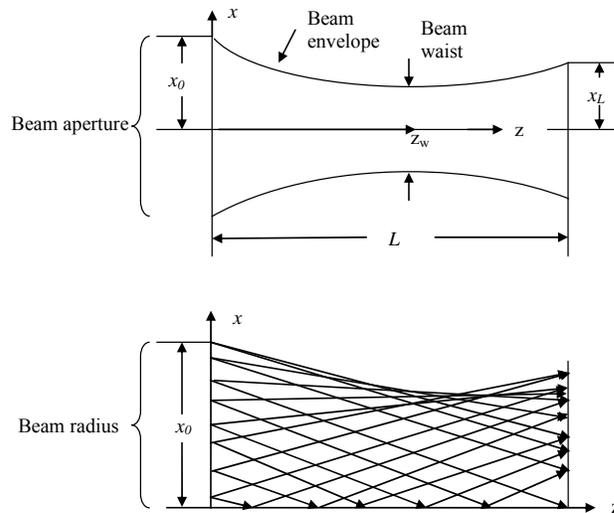


Figure 9. Beam envelope sketches. Upper: Beam projection in the drift region onto the x - z plane in configuration space. The beam propagates from the aperture at $z=0$ with an envelope parallel to the z -axis. The x - and y -directions are transverse to the z -axis. Lower: The beam envelope in the drift region is formed by a large quantity of particles traveling along straight trajectories.

To simplify the description of the beam parameters, the beam is referenced to the z -axis and the aperture is described as if it lies in the x - y plane. Other SDEF keywords, namely POS, AXS, and VEC, are employed to describe the location and orientation of the beam. These three keywords specify the center of the aperture, the beam direction, and the azimuthal orientation of the beam, respectively. This relationship is illustrated in Figure 10.

2.7.2 Example of Focused Beam Source

To illustrate the focused beam source feature, we model a 100-MeV muon beam with equal beam aperture half-widths, $x_0 = y_0 = 100$ cm, equal x and y normalized beam emittances, $\varepsilon_{nx} = \varepsilon_{ny} = 9.776 \times 10^{-1} \pi$ -cm-radians, and a drift region length of $L = 10^4$ cm. We define this beam as centered at the origin (POS=0 0 0) and pointed in the $+z$ -direction (AXS=0 0 1), with its

azimuthal orientation aligned with the x -axis (VEC=1 0 0). Figure 11 provides the required SDEF card and associates the keyword input parameters to the description and orientation of the beam.

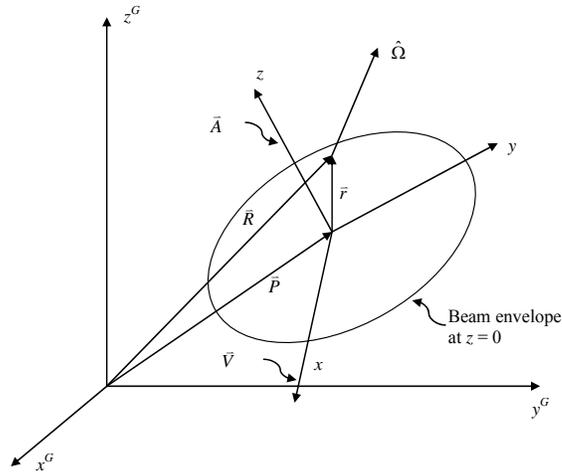


Figure 10. Locating and aiming a beam in MCNPX involves a transformation from local (x, y, z) to global (x^G, y^G, z^G) coordinates. The beam aperture is located in the local-coordinate x - y plane at the entrance to the drift region ($z=0$) at position \bar{P} (“POS”). The beam envelope is aligned in the direction \bar{A} (“AXS”) parallel to the $+z$ local-coordinate direction with the azimuthal orientation given by \bar{V} (“VEC”). Particle emission is in the direction $\hat{\Omega}$ at the local-coordinate position \bar{r} (the global position \bar{R}) as determined by beam parameters and Monte Carlo sampling.

Figure 12 shows a mid-beam side view ($y=0$), a view at the beam aperture ($z=0$), and a view at the $z=L$ for a cylindrical track-averaged (Type 1) mesh tally of the muon flux for transport in a void. The beam focusing effect is apparent. The cross-sectional beam flux profile varies as a function of axial location.

Similar views for the same beam transported in air are provided in Figure 13. Muon scattering in air induces a de-focusing effect.

```
SDEF PAR=| ERG=100 POS=0 0 0 AXS=0 0 1 VEC=1 0 0
BEM=9.776e-1 9.776e-1 1e4 BAP=1e2 1e2 0
```

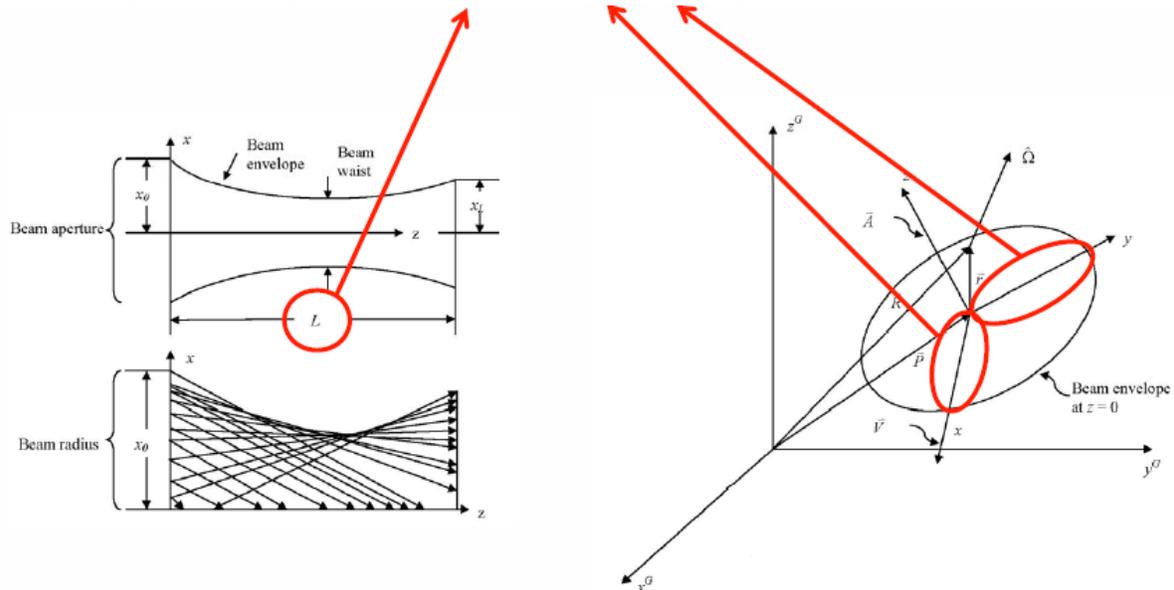


Figure 11. Description of a 100-MeV focused muon beam with a disk source positioned at POS=0 0 0 with a normal given by AXS=0 0 1 and an azimuthal orientation given by VEC=1 0 0. The desired drift-region length, L , is 100 m, and the beam aperture half-width in both the x - and y -directions is 1 m.

2.8 PTRAC COINCIDENCE OPTION

An option added to the PTRAC feature makes it easier to model multi-fold coincidence problems. When the new PTRAC output-control keyword, COINC, is used in conjunction with the TALLY keyword (which provides a list of tallies for filtering), COINC causes a list to be printed to the PTRAC file: When at least one tally is scored, all the tallies from that history along with the magnitude of their scores are printed.

Optional entries to the COINC keyword are available:

- COINC=[COL] Creates a full printing of all tallies specified, even if a tally had a zero score. Column-based output is provided. (Default)
- COINC=LIN Prints tally-score pairs for non-zero scores only.

When used in conjunction with the COINC keyword, TALLY entries must be positive. The existing VALUE keyword can be used to set threshold scores for the tallies itemized on the TALLY keyword. All scores below that threshold are treated as zero. The COINC keyword will force ASCII file output format (FILE=ASC or FILE=AOV). Note: The COINC feature only supports the TALLY and VALUE keywords as filter options.

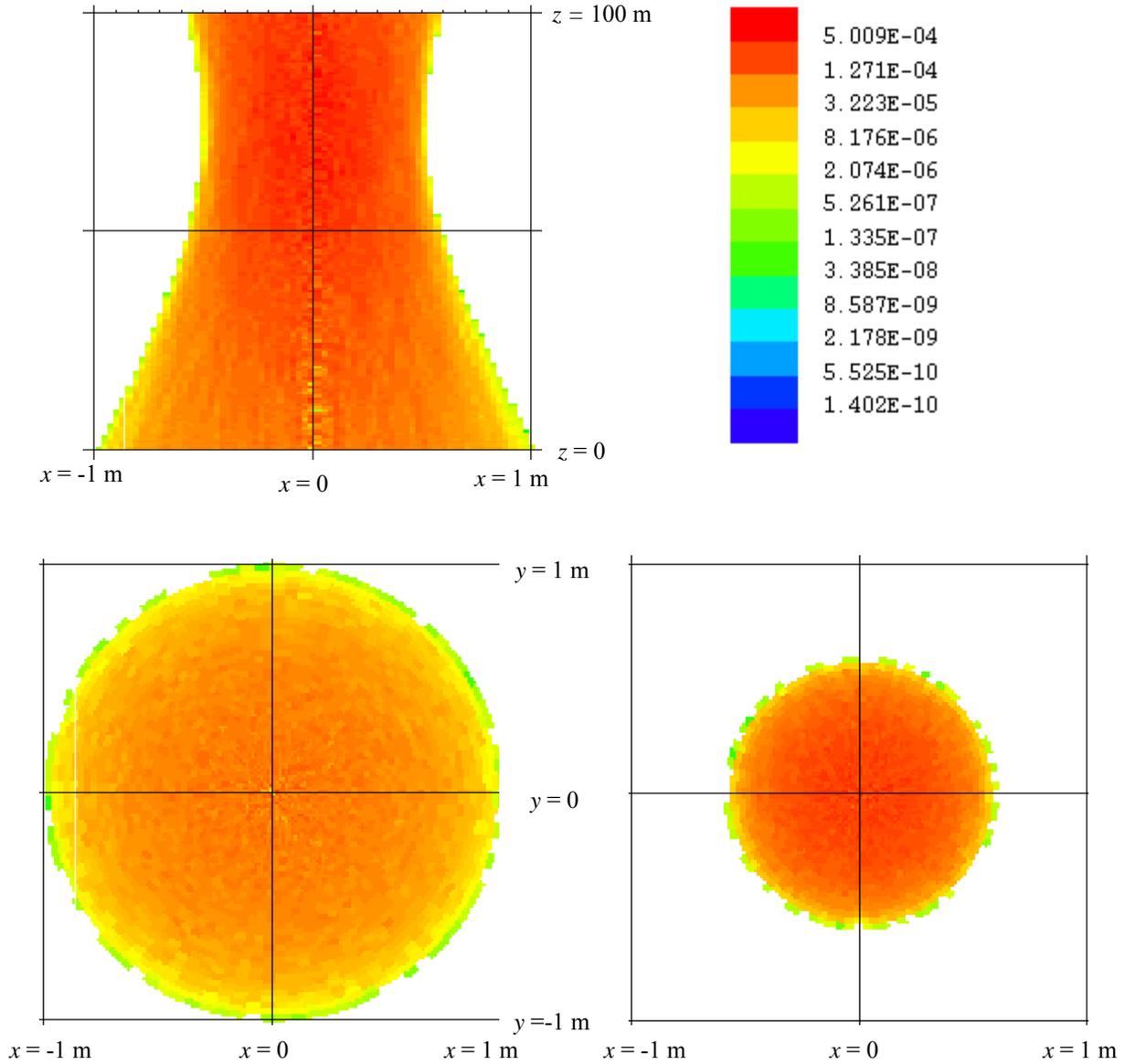


Figure 12. Mesh tally of the muon flux in a void. Upper: Mid-beam side view at $y=0$. Note that the window extent is exaggerated in the z -direction to better illustrate the beam axial profile. Lower left: Beam radial profile at the aperture ($z=0$). Lower right: Beam radial profile at the desired spot location ($z=L$).

2.9 LLNL MULTIPLICITY

2.9.1 LLNL Photofission Multiplicities

A photofission multiplicity code from Lawrence Livermore National Laboratory (LLNL) has been incorporated into MCNPX and is available for use. A 7th entry on the `PHYS:P` card, `fism`, controls selection of photofission multiplicity data either from the ACE libraries or the LLNL libraries:

- fism=0* sample photofission secondary (n,p) reaction from ACE libraries. (Default)
- fism=1* sample photofission secondary (n,p) reaction from LLNL libraries. When *fism=1*, photofission secondaries are sampled only when a photofission event occurs (unlike *fism=0*). This enables coincidence counting of photofission secondaries.

Figure 14 provides a comparison of ACE and LLNL photofission results for ^{235}U .

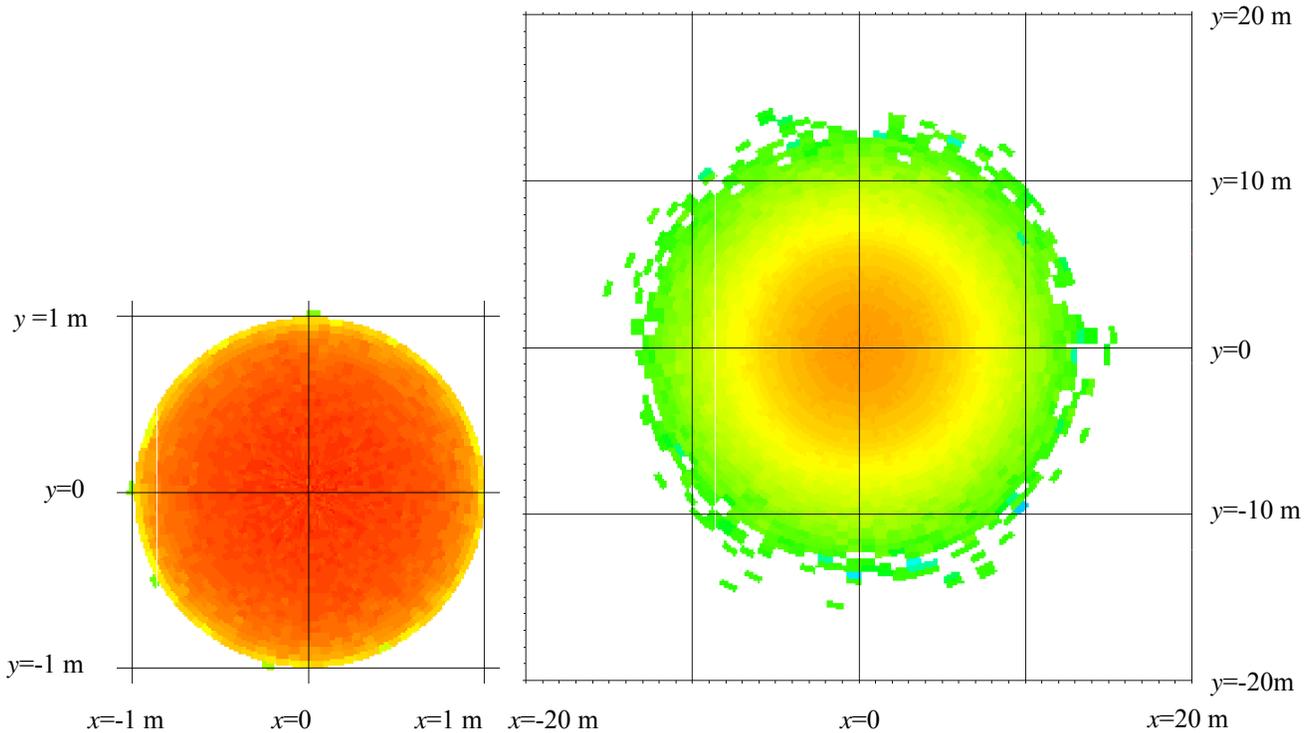
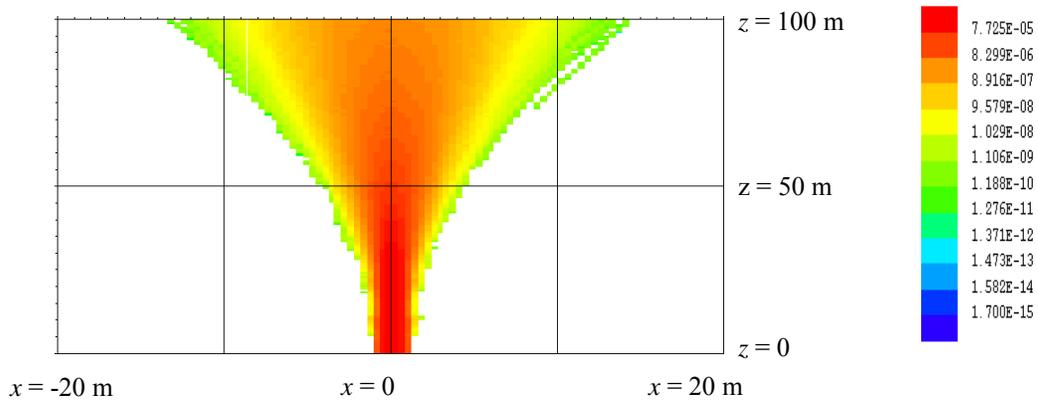


Figure 13. Mesh tally of the muon flux in air. Upper: Mid-beam side view at $y=0$. Note that the window extent is exaggerated in the z -direction to better illustrate the beam axial profile. Lower left: Beam radial profile at the aperture ($z=0$). Lower right: Beam radial profile at the desired spot location ($z=L$).

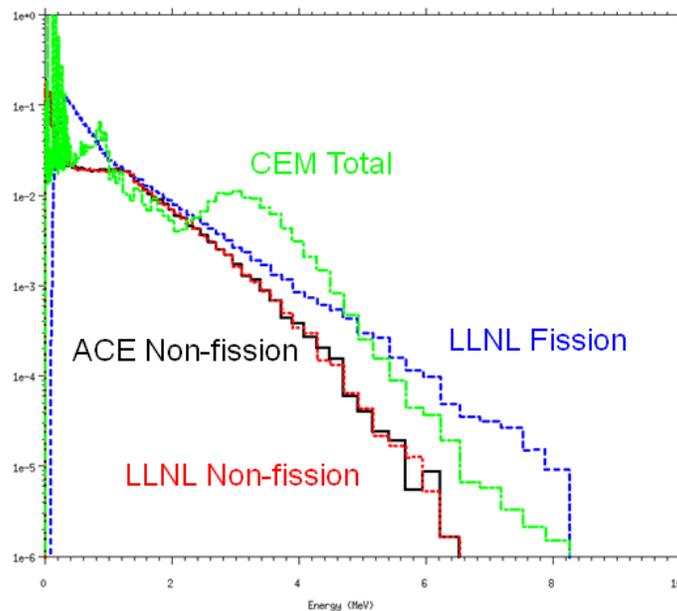


Figure 14. Resultant gamma-ray emissions from 12-MeV x-rays directed onto ^{235}U . Y-axis is the gammas/interaction/MeV/source particle. Note the deficiency of the ENDF VII photonuclear libraries that do not emit gammas from fission.

2.9.2 LLNL Neutron Fission Multiplicities

If the 6th entry on the `PHYS:N` card, `fism`, is set such that `fism=5`, then the LLNL treatment will be used for neutron-induced neutron and gamma fission multiplicity. Details of this multiplicity model can be found at the following web site: <http://nuclear.llnl.gov/simulation/>.

2.10 ARITHMETIC MCNPLOT OPTIONS¹

This developmental feature is not backed by the MCNPX cash awards quality assurance program. Users are encouraged to exercise this capability cautiously and report problems to the MCNPX development team.

2.10.1 Description

The MCNPX MCNPLOT plotting capability has been upgraded to include a new capability to post-process tally data using arithmetic operations. This capability facilitates addition, subtraction, multiplication, and division operations involving tally data. Also, several common functions now can be applied to tallies.

This feature involves the use of arithmetic operations to manipulate tally data that have been produced by one or more MCNPX calculations. This is a post-processing feature used with

¹ J. W. Durkee, et al., "MCNPX Graphics and Arithmetic Tally Upgrades," International Conference on Mathematics, Computational Methods, & Reactor Physics (M&C 2009), Saratoga Springs, New York, May 3-7, 2009.

MC PLOT. Thus, the arithmetic-operation commands are either entered by the user at the keyboard during an interactive MC PLOT session or via the contents of a COM file, such as the COMOUT file created during a previous plotting session. The arithmetic-operation commands cannot be included in an INP file. In this discussion, we refer to tallies created using post-processing arithmetic operations as “arithmetic tallies.”

Up to 1000 arithmetic tallies can be created during a MC PLOT session. These tallies can be input from multiple data files (RUNTPE or MCTAL files).

2.10.2 User Interface

New commands or keywords that now may be used with the MC PLOT tally plotting package include the following:

+	Add the tallies that appear on either side of the symbol
-	Subtract the tally that appears on the right of the symbol from that which appears on the left
*	Multiply tallies that appear on either side of the symbol
/	Divide the tally that appears on the left of the symbol by that which appears on the right
(and)	Parentheses used to combine addition or subtraction operations
=	Equate the tally name on the left side of the symbol to the tally expression on the right
WZMCTAL f_n	Read saved arithmetic tallies from file f_n ; if f_n does not exist, print an error message to the screen
RZMCTAL f_n	Write all saved arithmetic tallies that have been created in the MC PLOT session so far to file f_n ; if f_n already exists, create a new file with a unique name by changing the last letter of the filename of the new file to the next letter in the alphabet
PATALCMD	Print to the screen all saved arithmetic tally commands as well as the names of the MCTAL files from which the regular tally data were read; a similar listing of RUNTPE files is not yet supported
PRINTAL	Print to the screen both regular and saved arithmetic tally numbers
FONT f_1 f_2	Adjust the font size for plot axes (f_1) and for titles (f_2). The values of f_1 and f_2 can range from 0 to 1.
EXP	Exponentiation function
LN	Natural logarithm function
LOG10	Common (base-10) logarithm function
SQRT	Square root function
^	Powers function
INFINITY n	For arithmetic tallies, set non-physical, high bin values to the maximum value n .

Brief descriptions of these commands can be accessed via the MC PLOT “HELP” utility.

Several syntax rules apply to the commands associated with the arithmetic tally capability:

- If a product or quotient term contains only a single tally, no parentheses are required to enclose that term. However, if a product or quotient term contains an addition or subtraction term, then the term must be enclosed by parentheses.
- At least one space between the MCNPLOT `TAL` keyword and the tally number is required.
- Spaces between arithmetic-tally operators and the tally numbers are not required, but they are permitted to enhance visual interpretation.
- A quotient expression that contains multiple operations in the numerator and/or denominator requires the use of parentheses for the multiple terms.
- A command sequence can be continued to the following line using an ampersand (“&”) at the end of the line.
- There are no limits imposed on the types of regular tallies used in an arithmetic operation. For example, surface-integrated current (F1) and surface-averaged flux (F2) tallies can be added.
- The bin structure of regular and/or arithmetic tallies must be identical. Arithmetic operations involving tallies with different bin structure are disallowed.

Some of these usage rules will be clarified by the examples provided in Section 2.10.4.

2.10.3 Usage and Special Cases

Caution should be exercised when using the arithmetic tally capability. There may be instances when combinations of existing MCNPLOT commands for arithmetic tallies will fail. For example, the sequence in which a series of commands are entered may impact the calculated and plotted arithmetic tally results.

Some of the new capabilities include the following:

- Arithmetic tallies may be created and plotted with the option of saving the newly created tally.
- Saved arithmetic tallies may be used in subsequent operations.
- Tally input from multiple MCTAL files is allowed during a plotting session. The similar case of input from multiple RUNTPE files has not been tested.
- Saved arithmetic tallies may be written to and read from new auxiliary MCTAL files.
- An arithmetic tally may be created using an arbitrary number of tally additions or subtractions of regular or saved arithmetic tallies.
- Only a single multiplication or division operation involving either regular or saved arithmetic tallies is permitted to create a new arithmetic tally. However, multiple addition and/or subtraction operations can be used to form the product or quotient terms.
- The argument of each function operation (i.e., “EXP”, “SQRT”, etc.) must be a single tally—no operations are permitted within a function’s argument.
- If an operation is used to create a new tally, the operation itself is listed as a title line in the plot.

Unsaved arithmetic tallies are plotted as they are created, but are not available for later use. Saved arithmetic tallies are plotted as they are created and are available for use later in the plotting session. Saved arithmetic tallies must be assigned integer tally numbers between 0 and 9990 that end in zero (“0”).

The 8-dimensional tally array (“TAL”) contains tally data formed during the execution of an MCNPX calculation. Although extraction of the data from TAL is permitted to allow plotting of the data, TAL data itself cannot be altered. With the addition of the arithmetic-tally feature, this statement remains true; i.e., the regular tally data in the TAL array cannot be altered or corrupted by the arithmetic tally operations.

2.10.4 Examples

Example 1:

```
tal 28 / tal 8
```

This MCNPLOT command will plot the results of tally F28 divided by tally F8 for the currently specified RUNTPE or MCTAL file, but will not save the result.

Example 2:

```
tal 900 = ( tal 4 - tal 144 ) / tal 4
```

The regular F144 flux tally from the currently specified RUNTPE or MCTAL file is first subtracted from the F4 flux tally; this result is then divided by the F4 tally values. The final result is plotted and assigned to the arithmetic tally tal 900.

Example 3:

```
tal 0 = tal 2 fix f=1 + tal 92 fix c=2
tal 10 = tal 22 / tal 42
tal 20 = tal 0 - tal 10
```

Saved arithmetic tallies can be constructed using regular tallies, other saved arithmetic tallies, or a combination of both. The above MCNPLOT sequence constructs tal 0 and tal 10 from regular tallies and then saves the difference of tal 0 and tal 10 as tal 20.

Example 4:

```
rmctal=test_f1.m
tal 10 = tal 24 fix f=8
rmctal=test_f2.m
tal 20 = tal 24 fix f=8
tal 30 = tal 10 - tal 20
tal 40 = tal 10 + tal 20 + tal 30
```

In MCNPLOT, reading a new RUNTPE or MCTAL file will erase any previously read-in tallies. Assigning tallies to new ones ending in “0” will allow previously read-in information to be saved when new files are read. In the above MCNPLOT command sequence, regular tally data (F24 flux tallies) are input from MCTAL files created by two different MCNPX calculations. As each MCTAL file is read, the specified tally information is saved as an arithmetic tally with a unique user-defined tal number (i.e., tal 10 and tal 20). Finally,

using these two saved data sets, two saved arithmetic tallies (tal 30 and tal 40) are created.

Example 5:

```
rmctal=muon500_objnf_e9.m
tal 10 = tal 4 fix f=2 + tal 4 fix f=3
```

Tally information is read from a user-designated MCTAL file and tal 10 is created by adding the flux scores for the second tally cell of tal 4 to those for the third tally cell. The result is plotted in Figure 15. Unless overridden by user-specified title lines in MCPLLOT, the default title will be the operation line that creates the plot.

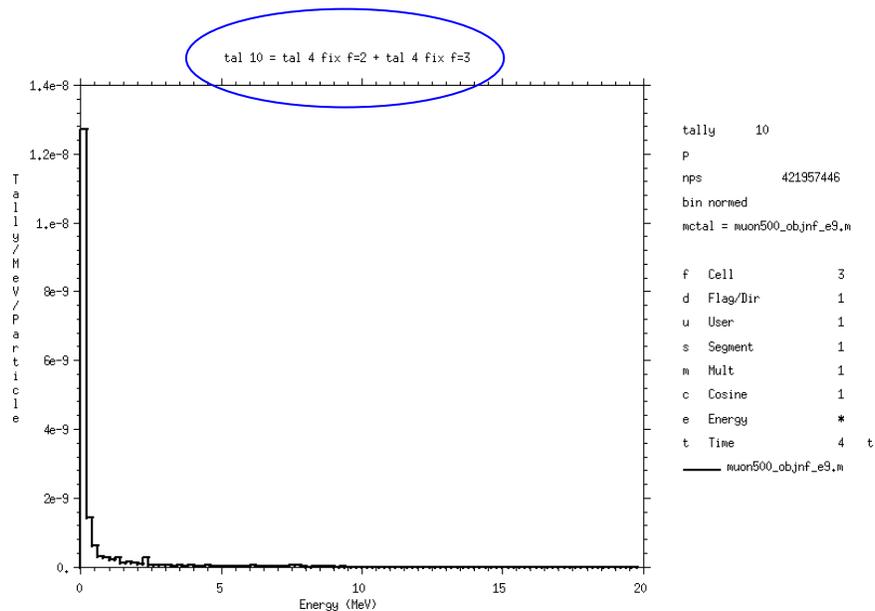


Figure 15. The title of this plot, circled in blue, is given by the default value: the operation that created the plot. This title can be replaced by using the `TITLE n` command available in MCPLLOT.

Example 6:

```
rmctal=pcpp1m
tal 0 = tal 1
rmctal=pcpp2m
tal 10 = tal 1
tal 30 = tal 10 - tal 0
legend 0.8 5.0
title 1 "New Arithmetic Tally Feature"
title 2 "Test of the Subtraction Feature"
font 0.7 0.7
tal 0 label "tal 0" cop tal 10 label "tal 10" cop tal 30 label "dif"
```

In this example, the respective F1 tallies from MCTAL files PCPP1M and PCPP2M represent coarse-bin, surface-integrated flux tallies for simulations assuming a 1-MeV and a 2-MeV point neutron source in water. The F1 tally from PCPP1M is saved in `tal 0` and the F1 tally from PCPP2M is saved in `tal 10`. The saved arithmetic tally `tal 30` represents the difference between `tal 0` and `tal 10`; all three arithmetic tallies are plotted in Figure 16. The commands used to create the plot below are provided for completeness.

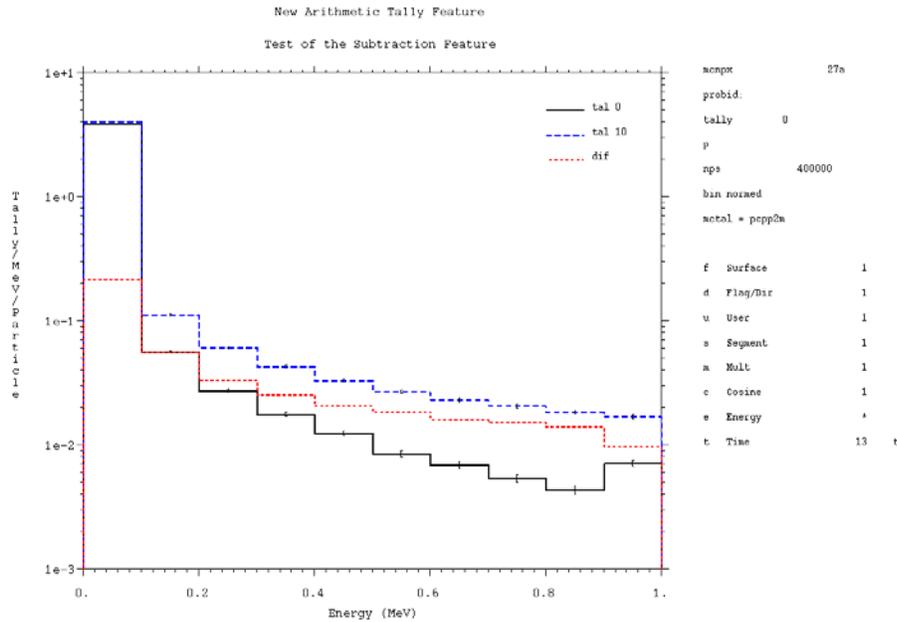


Figure 16. Three arithmetic tallies are coplotted, `tal 0`, `tal 10`, and `tal 30`, where `tal 30` is the red dotted line representing the calculated difference between `tal 0` and `tal 10`.

Example 7:

$$\text{tal 20} = \exp(\text{tal 1}) + \text{sqrt}(\text{tal 10})$$

In this example, the exponential of regular surface-integrated current `tal 1` is added to the square root of the saved arithmetic `tal 10`. The sum is stored in arithmetic tally `tal 20`. Note that the argument of each function must be a single tally—no operations are permitted within the argument of a function.

Example 8:

$$\text{tal 50} = \text{tal 22}^{-1}$$

`infinity 0`

The `infinity` command sets non-physical, large bin values to a stipulated value that is used for the post-processing of arithmetic tally data. The setting of the `infinity` parameter permits plotting of tally data while omitting non-physical noise. The default value of the `infinity`

parameter is $1e37$. In this example, if `tal 22` contains zero values in some tally bins, then addition of the `infinity 0` command will set the bin values that would have contained infinity in arithmetic tally `tal 50` to zero. The subsequent plot will appear more appealing and be easier to view.

2.11 RECEIVER-OPERATOR CHARACTERIZATION (ROC) TALLY OPTION

A new special tally option (`FT ROC`) separates tallies into two components, signal and noise. These tallies can then be summed over a batch of particles histories, along with details of their probability density functions (PDFs). Integration of these PDFs creates a Receiver-Operator Characterization (ROC) curve. The data for this curve is printed in a new output table (Table 163). The “signal” portion of a tally is identified using the first 8 entries on the associated `TF` card, while the “noise” portion is identified by the second 8 entries. (See Section 3.13.) During a calculation, the signal and noise tally values are saved for each batch of histories, as specified by the `nhb` parameter following the `ROC` keyword. These distributions of tally values are formed into signal and noise probability distribution functions (PDFs). Integration of the signal PDF (labeled as the Probability of Detection, PD) is plotted as a function of the integral of the noise PDF (labeled as the Probability of False Alarm, PFA), resulting in the printed ROC curve. A table of the PDF values is also provided in Table 163.

The entries for the `ROC` special treatment keyword are the following:

```
ROC nhb [m]
```

where

`nhb` is the number of histories per batch. This parameter is used to set the 5th entry on the `PRDMP` card (which sets the TFC frequency). This value should represent the total number of source particles emitted over the time interval of interest. The `WGT` keyword on the `SDEF` card should be set to the default value of unity. The `nps` value on the `NPS` card should be set to a multiple of `n`; the `nps` value will then be used to determine the number of sampled batches. We recommend that `NPS` should be 50–100 times the value of `nhb`.

The parameter `m`, which is optional, specifies the maximum number of batches that will be kept and analyzed. The default value is 100. We recommend `m` should be greater than 50 and perhaps two times the number of batches planned, even considering possible continue-runs. (This value cannot be increased in a continue-run file.) If there are multiple tallies with `ROC` entries, the maximum `m` value is used.

Example:

```
f1:n 1
t1 1e8 1e37
tf1 j j j j j j j 2 j j j j j j j 1
ft1 ROC 1000
```

In this example, tally `F1` scores the current of neutrons crossing surface 1. This tally is divided into two time bins, neutrons arriving before 1 second (i.e., 1×10^8 shakes) and those arriving after 1 second. The `TF` card associates the second time bin as the “signal” and the first as the “noise”. The signal and noise currents are accumulated for each batch of 1000

particle histories (the value is provided by the first entry after the ROC keyword). The resulting tally values are formed into signal and noise PDFs that are integrated and plotted in Table 163 as a ROC curve for this tally.

2.12 PULSE-HEIGHT LIGHT TALLY: TRIPLE AND QUADRUPLE COINCIDENCES

The pulse-height light tally (FT8 PHL) has been extended to enable tallying of triple and quadruple coincidences in addition to singles and doubles. (Please refer to the 2.6.0 MCNPX User's Manual for an explanation of the PHL keyword input format associated with the tally special treatment option FT.) The expanded entries for the PHL special treatment keyword are the following:

```
PHL      n  ta1 ba1 [ ta2 ba2 ... ]
          [ m  tb1 bb1  tb2 bb2 ... ]
          [ j  tc1 bc1  tc2 bc2 ... ]
          [ k  td1 bd1  td2 bd2 ... ]
```

where m , j , and k are the number of F6 tallies for the 2nd, 3rd, and 4th regions, respectively. The tally numbers and f-bin values for these regions work the same as for the first region.

2.13 TIME-DEPENDENT F8 TALLIES USING PULSE-HEIGHT LIGHT OPTION

The T (time bin) card is now allowed with pulse-height tallies (F8), but only when used in conjunction with the FT PHL option. In this case, the time-dependent energy deposition is taken from the associated F6 tally(s). If the time entries on the F8 card do not match those provided for the various F6 tallies, a fatal error is issued. If the associated F6 tallies do not have T cards, then one matching the F8 tally will be created internally.

Example:

```
f6:h      1
f16:t     1
f8:h,t    1
ft8       PHL  2 6 1 16 1  0
t8        10 20 30 40 50 60 70 80 90 100 1e37
```

In this example, the proton (F6) and triton (F16) energy depositions in cell 1 are combined into a pulse-height tally (F8) using the FT PHL option. The time-dependent behavior of these pulses is segregated into 11 time bins, 0–10 shakes, 10–20 shakes, etc. To obtain the time-dependent pulse shape, time-dependent energy depositions are obtained from the tallies identified by the PHL option. To accomplish this, the 11 specified T8 bins are applied to the associated F6 and F16 tallies with the creation of matching T6 and T16 cards (a warning message is generated when these cards are created).

3 MCNPX 2.7.D FEATURE EXTENSIONS AND ENHANCEMENTS

Some MCNPX features have been extended and have included changes or additions to the user interface. Where appropriate, initials of the principal developer(s) are provided in parentheses:¹

- spontaneous photon automatic weight adjustment (MRJ/LSW/GWM)
- burnup enhancements (MLF)
- lattice FILL error trap (JSH)
- Windows 64-bit support (GWM/MLF/MRJ)
- extension of ELC special treatment tally (JSH)
- RUNTPE initialization (GWM)
- LET tally (MRJ)
- ICRP-60 dose function (GWM/MRJ)
- residual tally upgrades (JWD/GWM)
- lattice cell rejection for sources (GWM)
- ACT card (GWM/JWD/MRJ)
- replacement of ²³⁵U delayed neutron spectrum (GWM)
- TF card extension (GWM)
- FM card extensions (GWM)
- contour legend added to geometry plotter (JWD/MRJ)
- muonic x-ray database expansion (ABM/GWM)
- heavy-ion recoils added to light-ion recoil (MRJ)
- improved delayed gamma spectra (JWD)
- delayed neutron and delayed gamma calculations using implicit capture (JWD)
- new photoatomic form factors (JSH)
- memory reduction options and bank size control for KCODE calculations (MLF)
- delayed particle speedup, accuracy improvement, and user control (JWD)
- updated output file format for PTRAC EVENT=CAP (JSH)
- full ZAID identifiers on MX card (MLF/LSW)
- nested READ card (MLF/LSW)
- NCIA upgrade (JSH)
- M0 library specification card (MLF/LSW)
- minor enhancements

¹ Joe W. Durkee (JWD, LANL, D-5), Jay S. Elson (LANL, D-5), Michael L. Fensin (MLF, LANL, D-5), John S. Hendricks (JSH, LANL, XCP-3); Michael R. James (MRJ, LANL, D-5), Russell C. Johns (RCJ, LANL, D-5), Gregg W. McKinney (GWM, LANL, D-5), Stepan G. Mashnik (SGM, LANL, X-3-MCC), Jerome M. Verbeke (JMV, LLNL), Laurie S. Waters (LSW, LANL, D-5)

3.1 SPONTANEOUS PHOTON AUTOMATIC WEIGHT ADJUSTMENT

The decay (or spontaneous) gamma source is a feature that allows the user to easily create a gamma spectra source associated with the decay of specified isotopes. With the implementation of the CINDER database and a gamma-line database, MCNPX can now lookup the appropriate activity and decay lines associated with a large number of isotopes. For many other isotopes, a multi-group treatment is available.

Spontaneous material source: The user can build a material that includes unstable isotopes and specify their appropriate fractions. In this case—analogue to the “SF” particle identification feature—the “SF” particle type can be specified on the SDEF card. The decay gammas will then be created based the unstable isotopes found in the material card at the sampled source location. If multiple unstable isotopes are present, they will be sampled based on their relative activities *within* that material.

Example 1:

```
m1  1001  1
    8016  1
    7016  1e-4      $ Unstable isotope N-16
    25054 1e-2      $ Unstable isotope Mn-54

sdef par=sp pos= 0 0 0  $ Location of material 1
ACT  DG=LINES
```

When the SF source is specified, the code will create an optional table 44 that summarizes the activities of the materials in the problem.

Spontaneous gamma particle specification: The other way to start decay gammas builds upon the heavy ion feature in MCNPX. The user can specify a $Z*1000+A$ as a particle type on the SDEF card and set the energy of that particle to zero. This will signal the code not to transport the heavy ion but to start its decay gammas. Note that in this case, the ‘#’ (heavy ion) *must* appear on the MODE card.

Example 2:

```
mode p #
sdef par=7016 erg=0 pos= 0 0 0
ACT  DG=LINES
```

Features and defaults: The decay gammas that are emitted are assumed to arise from the instantaneous activity of a large pool of decaying isotopes. So the time behavior will assume either whatever is specified on the SDEF card or the default of TME=0.

The sampled heavy ion isotopes will appear in Table 110 as the source particle although the created gamma lines do not.

It is also possible to do distributed sources with either of these options, with both options together or in combination with other sources in MCNPX.

As is the case with other source particles, be aware that if an isotope emits multiple gamma lines, the emissions will not necessarily be correlated.

Also note that isotopes with half-lives longer than 1×10^{18} seconds ($\sim 3.17 \times 10^{10}$ years) are treated as stable.

Exponential decay function: A new source probability function has been added that allows users to create a source with an exponential decay shape. The special function is invoked on the associated source probability (SP_n) card by a “-7” followed by the half-life specified in units of shakes. The default half-life is 1 shake.

Example 3:

```
sdef tme=d1
sp1 -7 2e8 $ 2e8 shakes = 2 seconds
```

SP_n W source probability option: A new source probability option has been added. The “ SP_n W” is a distribution specification that can only be applied to particle distributions. This distribution allows the user to specify actual intensities for a mix of particle sources. The intensities will be normalized per standard operation of the source, however the factor used to renormalize the intensities will be applied to the source weight to give the tallies the correct magnitude.

Example 4:

```
sil L n p h
sp1 W 3e9 5e9 2e9
```

The source shown here will create three sources and sample them by the relative magnitudes (neutrons 30%, photons 50%, and protons 20%). The weight assigned to each particle will be the sum of the non-normalized values, $3E9+5E9+2E9=1E10$.

The second aspect of the “ SP_n W” option is to allow SP (spontaneous photon) and SF (spontaneous fission) sources to be assigned magnitudes automatically in the code. A negative number corresponding to one of these two source types tells MCNPX to use the cell volume represented by the cell number that follows for the computation of the intensity.

Example 5:

```
sil L sp sf n
sp1 W -10 -15 3e9
```

In the source described here, the spontaneous photon source will look to cell 10 and use the material and volume to calculate the overall activity that will be substituted into the $SP1$ distribution. Correspondingly, the SF source will look to the material and volume in cell 15 for the intensity of the spontaneous fission source. (Note that a $+SF$ normalizes per spontaneous fission neutron, a $-SF$ normalizes per spontaneous fission.) The neutron source is unchanged.

Once the overall activity is computed, the renormalization will be done as before and the value passed into the weight parameter.

This option will also work with the *SB* (source biasing) option where sampling frequencies can be adjusted with the weights to bias the distributions.

If the cell specified in the *SPn W* option is a lattice cell, then the code may not know the correct volume for this cell. A volume can be supplied by a *VOL* card or with a *VOL* keyword on the cell card. If the user does not wish to correct the volume in these ways, a *WGT* keyword can be used with the source as a multiplicative factor.

Example 6:

```
sdef par=d1 wgt=264
sil L sf
spl w -35
```

In this example, the spontaneous fission source is weighted by the activity from cell 35, which has been duplicated 264 times in the geometry. The final source weight will be the activity from cell 35×264 .

3.2 BURNUP ENHANCEMENTS

Parallelizing the CINDER90 Interface: The burnup capability in previous versions of the code required that MCNPX calculate steady-state reaction rates (when transport cross sections were available) and 63-group fluxes to generate depletion coefficients for the time-dependent CINDER90 burnup calculation. Because MCNPX was already parallelized, the steady-state reaction-rate calculation was also parallelized in MCNPX 2.6.B to execute in multiprocessor mode. However, at the end of each steady-state reaction-rate calculation each slave processor had to rendezvous with the master processor to perform the interface/CINDER90 subroutines in a serial execution.

Several independent serial looping structures within the burnup interface allow the assemblage of depletion coefficients and isotopic information into a format suitable for CINDER90 execution. The computational expense associated with this serial execution increases with the number of burn materials requested in the burnup calculation. For example, burning a single material may only require one minute of interface/CINDER90 execution time; however, burning 150 materials may require 300 minutes.

Because the depletion of each burn material is an independent calculation, the computational cost associated with the interface/CINDER90 execution was remedied by parallelizing the interface/CINDER90 routines for multi-processor execution. The interface/CINDER90 calculation is now distributed across all available processors including the master processor. Each processor executes the interface/CINDER90 routines for a subset of burn materials and then rendezvous at the end of the interface/CINDER90 routines to determine total system burnup as well as atom densities for the subsequent reaction-rate calculation. Because the interface/CINDER90 routines are independent for each burn material and minimal communication across processors is necessary to execute the interface/CINDER90 subroutines, the computational enhancement scales almost linearly with the number of processors.

Variable Dimensioning for Burnup and Spontaneous Photons: The dimensions of spontaneous photon and burnup arrays were made variable so that these arrays only take up computer

memory space when they are used for these features. Certain arrays for the burnup and spontaneous photon capability were automatically dimensioned by the mix variable for any type of calculation. This unnecessary dimensioning wasted memory, thus limiting the size of calculations that could be examined by the code. All the arrays for the burnup capability are now dimensioned by unity if a BURN card is not present; similarly, all arrays for the spontaneous photon capability are dimensioned by unity if the spontaneous-photon capability is not used.

Unlimited CONC Changes: Additional dynamic dimensioning now permits an unlimited number of user-specified concentration changes (CONC option on BURN card.) Users implementing the MATMOD keyword in MCNPX 2.6.A(0) received strange results when trying to manually modify more than three nuclides per time step. Users may now manually modify as many nuclides as exist in the burn material. Nuclides that make up the burn material are included from the material card, fission product tier, and isotope generator algorithm.

3.3 LATTICE FILL ERROR TRAP

Errors in a fully specified lattice FILL are now captured with a “Bad Trouble” error. This is not a bug fix because it only happens with user errors when setting up geometries. Previously, an erroneous lattice fill would go undetected and usually cause a crash or lost particles, but occasionally cause wrong answers.

Consider the following:

```
FILL  0:2  0:1  0:0  1  1  1  1  1  1  2
```

The fully specified FILL describes a 3×2×1 lattice, so it should be followed by six universes. Instead there are seven. The lattice fill error trap now detects either too few or too many universes.

3.4 WINDOWS 64-BIT SUPPORT/COMPILATION WITHOUT GRAPHICS

MCNPX may now be built without graphics on Windows (using both Intel 9.1 and 10.1) for MPI parallel versions. The MCNPX C code was revised to omit the use of TIMEVAL and GETTIMEOFDAY() and to use instead the C++ intrinsic function FTIME. This revision eliminates the need for MCNPX to use timing calls in X11 libraries and allows for compiling on Windows 64-bit systems.

3.5 SPECIAL TREATMENT TALLY FOR ELECTRON CURRENT

The FT special tally treatment ELC option discriminates between positively and negatively charged particles, segregating them into separate bins. The capability now has been extended to neutral particle/antiparticle pairs. Suggested by Piero Neuhold, ANSALDO, Genoa, Italy.

3.6 RUNTPE INITIALIZATION DURING MPI

When running MCNPX with MPI, the code attempts to use the RUNTPE file to initialize all daughter processes. The master will write the RUNTPE file with the information necessary to initialize the problem. The daughter processes will then read that RUNTPE file for initialization rather than receiving that information through MPI message passing. This is only possible when using a shared file system. This method can bypass some problems with message passing that

can cause the buffer to overflow. If the daughter processes cannot locate the RUNTPE file, the old method of message passing is used to initialize them.

3.7 NEW SPECIAL TREATMENT TALLY: LET

The special tally treatment using `FTn LET` can now be applied to track length tallies to record flux as a function of stopping power instead of energy. When the `FTn LET` option is specified, the values specified in the energy bins are interpreted as stopping power values with units of MeV/cm. This option can only be applied to charged particle tallies.

Example:

```
fc4      Proton flux LET
f4:h     77
e4       1e-2 99ilog 6e4
ft4      LET
```

This example is a tally that records the proton flux in cell 77 for an LET tally. The tally results are recorded in 100 bins of stopping power from 0.01 to 60000 MeV/cm.

3.8 SPECIAL DOSE FUNCTION

An ICRP-60 effective-dose conversion function was added that applies to energy deposition tallies and provides the dose in units of Gy or Rad. This effective-dose function uses a lookup of the stopping power to create a multiplier of the absorbed dose. To request this dose function, specify `IC=99`, `IU=1`, and `FAC=-3` on the `DFn` card. A table is provided for neutrons, which have no stopping power. Other neutral particles would need to have energy deposition modeled through charged particles for accurate effective-dose tallies. Lookup is performed using the appropriate charged particle stopping power (or a lookup table for quality factor for neutrons) as shown in the following equation:

$$\bullet \quad Q_{ICRP-60}(S(E,p)) = \left\{ \begin{array}{ll} 0 < S(E,p) \leq 10 & Q_{ICRP-60} = 1 \\ 10 < S(E,p) \leq 100 & Q_{ICRP-60} = 0.32 \times S(E,p) - 2.2 \\ 100 > S(E,p) & Q_{ICRP-60} = \frac{300}{\sqrt{S(E,p)}} \end{array} \right\} .$$

where $S(E,p)$ is in $\frac{keV}{\mu m}$

Example:

```
fc6      Helium-4 (alpha) dose equivalent (Sv)
f6:a     77
df6      ic=99 iu=1  fac=-3
fm6      1.6021e-10  $ F6 MeV/g * 1e6 eV/MeV * 1.6021e-12 ergs/eV
                    $ * 1 Rad/100ergs/g * 1 Gy/100 Rads
                    $ * QF = F6 in Sv
```

This example uses a combination of the ICRP-60 dose function and an FM multiplier to produce a tally that gives results in Sv/source for alpha particles in cell 77. Note that the source strength must still be taken into account.

3.9 RESIDUAL TALLY UPGRADES

Significant improvements have been made in the way MCNPX handles residual tallies. The `FT RES` special tally feature, previously limited to residuals produced from the interactions from physics models, now accumulates residuals produced from neutron library interactions as well. In addition, the `FT RES` feature now works the same way for both standard `F` tallies and `F8` tallies. Specifically, the user may provide a list of cells for which residual tallies are desired; a list of specific ZAIDs is allowed as well.

Beginning with version 2.7.B, the `FT8 RES` card yields a list of residual nuclides produced by neutron-induced fission and activation reactions. The residual tallies can be obtained either with or without the emission of delayed neutrons and/or delayed gammas. Residual tallies can be obtained for analog or nonanalog (implicit capture) neutron transport.

For models that include light-ion recoil and the neutron capture ion algorithm (NCIA) (activated using the 7th entry on the `PHYS:N` card), reaction residuals are now included in the `FT8 RES` tally. In most instances, reaction residuals are determined using the ENDF reaction specifications for simple-multi-particle reactions. In rare instances, e.g., neutron bombardment of $^{10}\text{B}(n,t2\alpha)$, the ENDF reaction specifications can result in only light-ion production. In such cases, the heaviest light-ion residual is selected.

Version 2.7.D includes the capability to tally residuals on a cell-by-cell basis. Residuals may be tallied for models containing individual cells or repeated structures for either all cells or a subset of cells.

Example 1:

```
F8:#  1 100 T
FT8   RES 25 27
```

The entries on the `F8` tally card are cell numbers for which residuals are to be tallied. In this example, residual tallies are requested for cell 1, cell 100, and for cells 1 and 100 combined. The entries on the `FT8 RES` card specify the range of possible Z -values for which to tally the residuals. Here, residuals with atomic numbers between (and including) $Z=25$ and $Z=27$ will be scored.

Example 2:

```
F8:#  1 100 T
FT8   RES 25054 25055 25056 26055 26056 26057 27056 27057 27058
```

The entries on the `F8` tally card are cell numbers for which residuals are to be tallied. In this example, residual tallies are requested for cell 1, cell 100, and for cells 1 and 100 combined. The entries on the `FT8 RES` card specify a list of isotopes for scoring residuals. Production for specific isotopes of Mn, Fe, and Co will be included for this `F8` tally.

3.10 LATTICE CELL REJECTION FOR SOURCES

A range of lattice indices may be specified to produce a uniform sampling among those lattice elements. This enhancement still requires the use of a fully-specified `FILL` card for the listed lattice cell. The sampling is accomplished using rejection on all possible lattice elements. The `SDEF` keyword `EFF` may need to be decreased to accommodate sampling of a small portion of a large lattice.

Example:

For a lattice that has been defined with a fully specified `FILL` card, the following may be used to create source particles in a subset of that lattice using ranges specified for the lattice elements:

```
sdef cel=d1
si1  L (4<2[-1:1 -2:2 -3:3]<1)
sp1      1 104r
```

3.11 ACT: ACTIVATION CONTROL CARD

The new `ACT` card controls the delayed neutron/delayed gamma (DNDG) feature by particle type (options are currently limited to `N` for neutron and/or `P` for gammas) and the choice of fission (`FISSION`) or non-fission (`NONFISS`). Additional keywords added in v.2.7.D provide a convenient user interface to control the DNDG feature. The new keywords include `DN`, to choose use of libraries, models, or a combination for delayed neutrons (previously controlled using the 4th entry on the `PHYS:N` card); `DG`, to select line vs. multigroup data for delayed gammas (previously controlled using the 6th entry on the `PHYS:P` card); `THRESH`, to specify the fraction of gammas that are retained; `DNBIAS`, to establish delayed neutron bias (previously controlled using the 4th entry on the `PHYS:N` card); and `NAP`, to specify the number of activation products saved. The form of the card is

```
ACT  KEYWORD(s)=value(s)
```

where the allowed keywords with their respective options are

```
FISSION=[ NONE | N,P,E,A | ALL ]
NONFISS=[ NONE | N,P,E,A | ALL ]
DN=[ MODEL | LIBRARY | BOTH | PROMPT ]
DG=[ LINES | MG | NONE ]
THRESH=t (where t, is the fraction of gammas kept; default=0.95)
DNBIAS=n (where n neutrons/interaction is specified as a bias; default=analog calculation)
NAP=n (where n is the number of activation products saved; default=10)
```

The particle list can include one or more particle types. The “E” (beta) and “A” (alpha) entries are currently read in but these delayed particles are not yet produced. Use of the `PHYS:N`, 4th entry, and the `PHYS:P`, 6th entry, to control these capabilities results in a warning message of future deprecation. Caution: To avoid the selection of conflicting parameters, the user should not use both methods for specifying these options.

3.12 REPLACEMENT OF ^{235}U DELAYED NEUTRON SPECTRUM

Previously, through version 2.7.B, MCNPX used a ^{235}U spectrum for all delayed neutrons except for the following precursor nuclides, which had their specific energy values in the code: N-17, N-18, C-16, C-17, C-18, B-13, B-14, Be-12, and Li-9.

Now, a new delayed-particle library has been created, allowing a unique delayed neutron spectrum to be sampled for each residual. A warning is issued when no delayed neutron data are available and a residual with a non-zero delayed-neutron probability is sampled.

This feature is on by default and used automatically for delayed neutron problems.

3.13 TALLY FLUCTUATION (TF) CARD EXTENSION

Two sets of eight space-delimited entries are now allowed on the tally fluctuation (TF) card. Each of the eight entries corresponds to a specific FDUSMCET bin or group of bins. The first set of entries is associated with a tally signal component and the second with a tally noise component. (See the FT ROC option description in Section 2.11.) Furthermore, the TF entry format has been expanded to allow four forms:

- entry specifying a single bin
Example: 10
- entry specifying a range of bins:
Example: 10-12
- entry specifying a list of bins,
Example: 10,11,12
- entry that specifies a combination of a range of bins and a list of bins:
Example: 10-12,13,14

Example:

```
TF1    2 j 10-12,13,88 1-2 j 7,8,9 1-99 2    j 1 j j 2 j j j
```

Note that spaces are not allowed within a comma-delimited list of bins and/or bin ranges. Spaces continue to be used to delimit the 8 bin-type entries. The first 8 entries specify the bins that constitute the signal component of the tally, while the second 8 entries specify the bins that constitute the noise component of the tally. (The first bin listed in each entry will be used for generating the TFC output.)

3.14 FM CARD EXTENSION

A special FM tally option has been added that multiplies multiplicities by the principal interaction cross section. This option only makes sense when used with the LCA NOACT=-2 option.

If the parameter k on the FM n card is set to -3, the tally will be multiplied by the microscopic cross section of the first interaction. This option can be used with the LCA NOACT=-2 option to convert multiplicities into secondary production cross sections (with units of barns). This option works for all incident particle types except electrons; however, for charged particles caution

should be exercised because for some charged particles maximum cross sections are used instead of actual cross sections.

3.15 GEOMETRY PLOTTER: CONTOUR LEGEND ADDITION

A contour plot legend can be displayed for a mesh tally created using the geometry plotter. The legend can be turned on/off by clicking the “LEGEND” option in the interactive plotter. The legend will display the association of the color key to the numerical values in the plot. Some output of the interactive plotter will be suppressed to make room for the legend. There is no keyword command for this option.

3.16 EXPANSION OF MUONIC X-RAY DATABASE

The muonic x-ray database has been expanded to include all stable isotopes. This expansion was accomplished through use of the MUON/RURP code package. Although for many isotopes, the necessary nuclear data was not available to allow a precise calculation of the muonic x-ray spectra. For this reason, literature data is always the used for a given isotope when it is available. On the muon physics (PHYS: |) card, a seventh entry, *xmurnum*, has been added to control the selection of muonic x-ray data:

<i>xmurnum</i> =-1	use only x-ray literature data (isotopes without literature values do not emit muonic x-rays)
<i>xmurnum</i> =1	emit all x-rays, including data from the literature and from MUON/RURP (Default)

3.17 HEAVY-ION RECOIL

The light-ion recoil feature has been extended so that elastic collisions from neutrons and protons that occur in the library physics regimes now create heavy-ion recoils when heavy ions are specified on the MODE card. To illustrate this physics enhancement, ⁵⁶Fe elastic recoils from 20-MeV neutrons are tallied and displayed in Figure 17.

3.18 EXACT ENERGY INTEGRATION IMPROVES DELAYED GAMMA SPECTRA^{1,2}

Recall that equating the DG keyword on the ACT card to LINES (or, equivalently, the 6th entry on the PHYS:P card, *dgb*, to -102) invokes sampling of delayed gammas using models based on line-emission data augmented by 25-group data from the CINDER90 database.

The Monte Carlo paradigm for delayed gamma simulation involves the construction and sampling of cumulative distribution functions (CDFs) for each fission or activation event, including delayed-gamma-emission energy and time. The energy integral is evaluated according to the energy-CDF integration option and the availability of data. The energy-CDF integration technique has been improved. The improved strategy evaluates the energy integrals on an

¹ J. W. Durkee, et al., "Delayed-gamma signature calculation for neutron-induced fission and activation using MCNPX, Part I: Theory," *Progress in Nuclear Energy*, **51**, pp. 813-827 (2009)

² J. W. Durkee, et al., "Delayed-gamma signature calculation for neutron-induced fission and activation using MCNPX, Part II: Simulations," *Progress in Nuclear Energy*, **51**, pp. 828-836 (2009)

individual emission-line basis (i.e., “exact integration”) when possible. This serves to improve the fidelity of energy spectra when compared to preceding code releases.

In order to speed execution, coding has been developed to calculate core components of the CDFs once and store them for reuse. Among other things, this coding serves to reduce the number of CINDER90 invocations. However, competing against the streamlined-execution objective are storage issues associated with the sheer size of the arrays required to store CDF data.

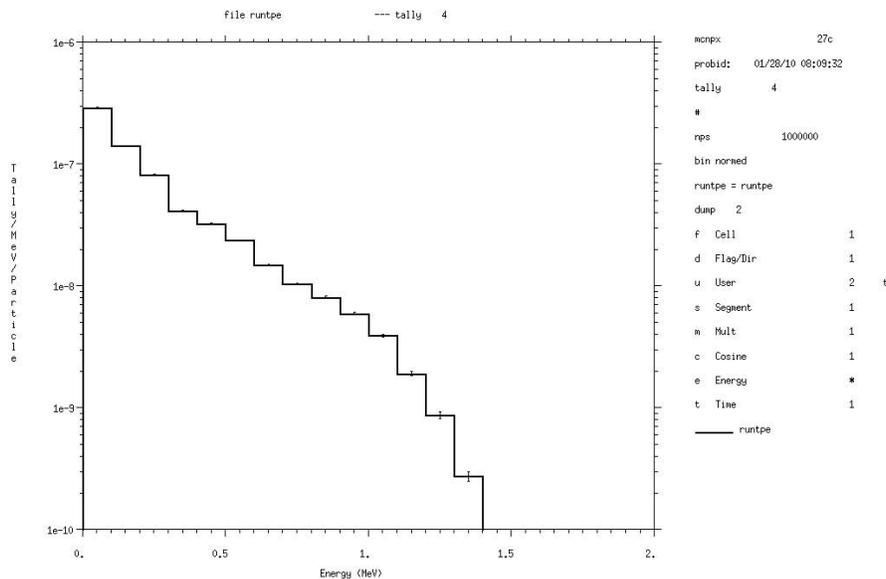


Figure 17. Flux tally of ^{56}Fe elastic recoils from 20-MeV neutrons.

Two workarounds have been developed and implemented to mitigate the impact of the storage and execution issues associated with the exact execution option: (1) CDF storage for the most often sampled fission products, and (2) fine-bin integration for fission or residual events producing lengthy decay chains.

MCNPX CDF storage has been tailored to treat the most often sampled fission products involving uranium and plutonium. Testing has shown that 345 fission products constitute over 99% of the most frequently sampled fission products. The identities of these fission products created by thermal fission of ^{235}U and ^{239}Pu [†] have been stored in arrays in MCNPX. Energy CDF calculation for the rarest (sub-1%) fission products would require recalculation for each sampling event, including calls to CINDER90. By ignoring the least-sampled fission products, execution

[†] Currently, MCNPX checks the input data for ^{235}U and ^{239}Pu . If either of these nuclides is present, then the pertinent fission-product-array data are used. For other fissioning nuclides, the data for ^{235}U are used. A future upgrade will address problem-dependent generation of the most-frequently sampled fission products.

time is reduced by >90%. Because of storage limitations, we do not allow the user to request the sampling of all fission products.

The size of the storage array corresponds directly to the number of emission lines that exist for a fission or residual event. Energy fidelity is directly impacted by the number of lines that can be treated. Testing has shown that many fission-product decay chains have tens to a few hundred emission lines. On the other hand, activation (rather than fission) products of uranium or transuranics have lengthy decay chains with tens of thousands of emission lines. MCNPX delayed gamma simulations can be executed on many modern platforms while allowing storage for up to 400 emission lines. Consequently, the energy-CDF integral can be done exactly on a line-by-line basis where there are 400 or fewer emission lines. However, when the storage allowed for emission lines is exceeded, some approximation to the energy integral must be made. For these cases, a fine-fixed-bin integral evaluation is performed. A bin structure is created based on the number of emission lines, and the energy-CDF integral in each bin is evaluated using all lines within each bin. For bins with only a single peak, the calculated emission is exact. For bins with two or more peaks, the fine-fixed-bin integration technique smoothes the peaks structure by reducing the amplitude of the high peaks and boosting the amplitude of the low peaks. The limit in the MCNPX code on emission-line storage is set internally.

CDF evaluation using exact integration can be done only when line data are available for a nuclide on the cindergl.dat file. When line data are not available for a nuclide, the CDF contribution must be evaluated using 25-group data and CDF integrals must be evaluated to properly account for the contribution. Line-emission data are available in cindergl.dat for 979 nuclides. For these nuclides, the new exact integration process preserves sampling of prominent lines. For the remainder of the 3400 nuclides treated by CINDER90, 25-group data must be used. The treatment of line of 25-group data is performed automatically by MCNPX.

Delayed-gamma spectroscopic results from HEU and ^{239}Pu fission induced by thermal neutrons are in good agreement with measured data. A comparison of data and simulation can be found in Durkee's "Delayed-gamma signature calculation for neutron-induced fission and activation using MCNPX, Part II: Simulations," referenced previously.

Please note that simulations involving delayed gammas cannot be executed using continue runs. Future upgrades are necessary to enable continue runs for input cases that require delayed gammas.

Delayed gamma sampling using the multigroup method and the exact sampling method are compared in Figure 18.

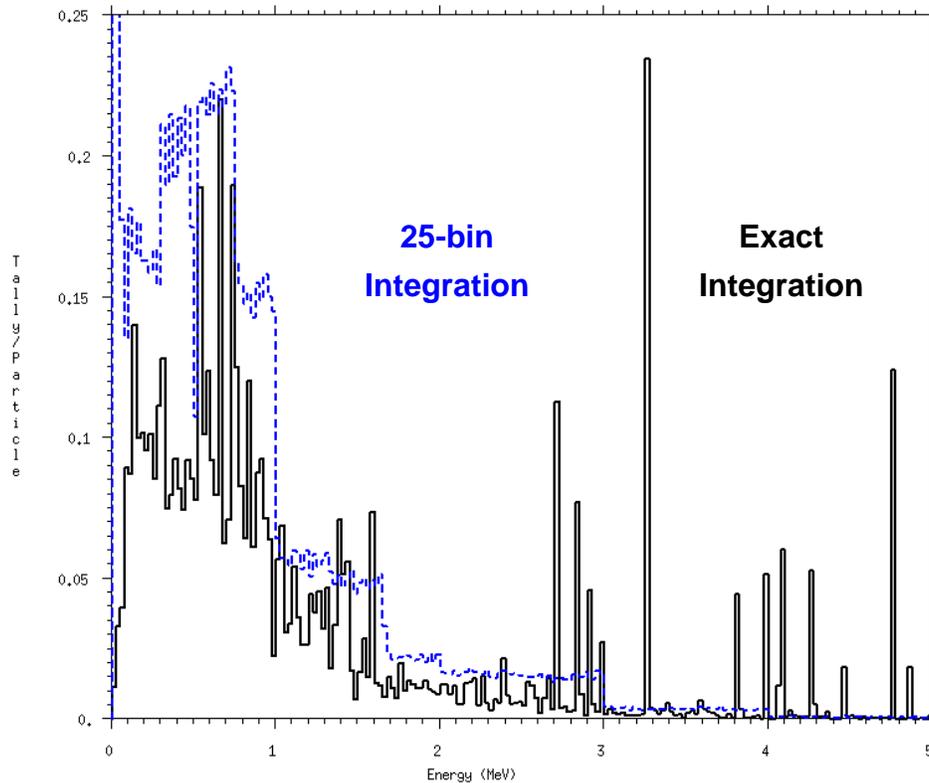


Figure 18. Delayed gamma spectrum emitted from ^{235}U struck by thermal neutrons. The delayed spectrum using a multigroup sampling method (ACT DG=MG) is compared to that using exact delayed-gamma sampling (ACT DG=LINES).

3.19 DELAYED NEUTRON/DELAYED GAMMA CALCULATIONS USING IMPLICIT CAPTURE

Previous to version 2.7.B, simulations involving neutron-induced reactions with delayed neutron and/or delayed gamma production using models had to be executed using analog capture. Since version 2.7.B, these simulations can be executed using implicit capture. Therefore, DNDG calculations involving neutron-induced reactions now can be conducted using the default (implicit capture) variance-reduction technique.

To invoke delayed neutron and/or delayed gamma production, use the ACT card (see Section 3.11). For implicit capture, no additional user input is required. To specify analog capture, set the 3rd entry on the CUT:N card to 0.

3.20 NEW PHOTOATOMIC FORM FACTORS

MCNPX 2.7.C treats photoatomic form factors for coherent and incoherent scattering according to the 40-year-old formulation predating MCNP. Rayleigh scattering form factors are tabulated in ACE files for a pre-defined array of 22 momentum transfer values for incoherent scattering and 55 momentum transfer values for coherent scattering. In this formulation, the maximum momentum transfer allowed is 6 \AA^{-1} . For the scattering of a 2-MeV photon, this limit restricts the angle of scattering to no more than 5.01 degrees. This is a non-physical cutoff. For scattering of

2-MeV photons off of high-Z materials such as uranium, approximately 20% of all Rayleigh scattering events result in photons scattered into higher angles. ENDF/B-VII photoatomic evaluations included form factors for momentum transfers up to $1e11 \text{ \AA}^{-1}$.

The new MCPLIB05 photo library is MCPLIB04 modified to provide the complete form-factor data available in ENDF/B-VII. The complete ENDF data are utilized; backwards compatibility is maintained by using the old hard-wired tables when the length of the incoherent scatter data equals 22. This library and the associated XSDIR entries are available from the MCNPX web site, <http://mcnp.x.lanl.gov>.

Note that using the entirety of the coherent and incoherent scattering form-factor data does not fully model photon elastic scatter. Nuclear resonance fluorescence, nuclear Thomson scattering, Delbruck scattering, and anomalous scattering factors remain omitted from MCNPX.

3.21 MEMORY REDUCTION OPTIONS AND BANK SIZE CONTROL FOR MODE N P E CALCULATIONS

Physics models can be disabled and memory not allocated to them by setting the neutron table/model cutoff energy above the maximum neutron energy. Note that this will only work for MODE N P E and when the photonuclear option is not invoked.

Example:

```
phys:n 15 3j 17
```

The neutron table/model cutoff energy is set to 17 MeV, which is greater than the specified maximum neutron energy (15 MeV). This combination invokes the memory-saving option.

Setting the neutron table/model cutoff energy greater than the maximum neutron energy also reduces the maximum number of secondary particles that can be stored in the particle bank. This reduction in the maximum quantity of secondary particles in turn reduces the amount of memory that must be allocated to the particle bank. For nuclides containing tabular cross-sections, the particle bank also stores unresolved resonance data for each secondary particle generated. Therefore, reducing the number of secondary particles stored in the bank significantly reduces the amount of memory allocated for these arrays.

MCNPX stores the following maximum number of secondary particles depending on problem type:

1. Default: 2048
2. Memory saving option: 128
3. >5 GeV/nucleon source: 16384

The user may also set the maximum quantity of secondary particles depending on problem type using the 22nd entry on the DBCN card.

3.22 DNDG SPEEDUP, ACCURACY IMPROVEMENT, AND USER CONTROL

The MCNPX delayed gamma (DG) feature has been upgraded to improve execution speed,¹ improve the accuracy of the calculated results, and provide the user with increased control of DG features.

3.22.1 Delayed Gamma Execution-Time Reduction

MCNPX DG simulations are computationally time and memory intensive. Improvements in the calculation and storage algorithm for the cumulative distribution functions (CDFs) have resulted in reduced execution times for calculations using multigroup (ACT DG=MG) or line (ACT DG=LINES) options. For line-mode cases involving activation, the upgrades result in significant execution speedup.

Code modifications affecting the multigroup execution mode (ACT DG=MG) cause CDFs for all fission and activation products to be calculated once and then stored for reuse. This coding improvement does not require user action. Incorporation of these modifications results in execution-time reductions of at least 95% for most multigroup-mode calculations that involve fission and/or activation reactions.

To achieve speedup of the line execution mode (ACT DG=LINES), a dynamic-list capability was implemented in MCNPX for activation products (i.e., residual nuclides). This capability enables the code to determine automatically the problem-dependent list of most frequently sampled activation products. CDFs for the most frequently sampled activation products are calculated and then saved for reuse. Implementation of these modifications results in execution-time reductions of over 75% for most line-mode calculations involving activation reactions.

By default, the number of activation products for which CDFs will be calculated once and stored for reuse is 10. This top-10 list of the most frequently sampled activation products is updated dynamically during problem execution. The user may change the number of activation products for which CDFs are stored by assigning a different value to the NAP keyword of the ACT card. (Refer to Section 3.11.) If the user's computer contains adequate storage for the user-requested NAP value, then execution will proceed. If not, the NAP value must be reduced by the user. In general, if the value of NAP is greater than or equal to the actual number of activation products created in the problem, then the CPU time is minimized for line-mode execution of models involving activation.

If activation is not desired, then we recommend you do not use the ACT NONFISS option.

In line execution mode, fission and activation are treated separately. For fission calculations, a static list of 125 fission products is used. This list includes the most frequently sampled fission products that are generated when ²³⁵U and ²³⁹Pu are subjected to thermal-neutron fission. No user control for fission exists in MCNPX.

¹ J. W. Durkee, et al., "MCNPX Delayed-Gamma Feature Enhancements," Los Alamos National Laboratory report LA-UR-10-03383 (2010)

3.22.2 Improvement in Delayed Neutron/Delayed Gamma Emission-Spectra Accuracy

Accuracy of DNDG-calculated results has been improved through upgrades to the integration algorithm for the CDFs. Earlier code releases used the trapezoidal rule algorithm to perform time integration of the CDFs.¹ MCNPX 2.7.D uses analytic results for line-mode models when the fission or activation event results in the creation of a single DG emitter. Details of the new CDF time-integration scheme can be found in Appendix A of this document.

3.22.3 User-Control of Maximum Delayed Neutron/Delayed Gamma Emission Time

To reduce the CPU time for a DNDG calculation, the user may now control the maximum time allowed for DNDG emission by using the CUT card(s). The default (and maximum) emission time for DNDG emission in MCNPX is 10^{10} s. By using the CUT card(s), the maximum DNDG emission time becomes (1) the neutron or photon time cutoff if either particles' time cutoff is provided, or (2) the minimum of either the neutron or photon time cutoff if both neutron and photon time cutoffs are provided. The use of the time cutoff reduces the number of times at which the CDFs are calculated, but not the specific times at which the CDFs are calculated, up to the time cutoff.

In summary, use the CUT:N and/or CUT:P card(s) to limit the maximum emission time for DN and/or DG to less than 10^{10} seconds.

Example:

```
CUT:N  1.0d16  j  0  0
CUT:P  1.5d15  j  0  0
```

Delayed neutron and delayed gamma emission will be calculated to 1.5×10^7 s, the lesser of 1.0×10^{16} and 1.5×10^{15} shakes.

3.22.4 Warnings and Notations Regarding DNDG Emissions

A warning message has been added to alert the user when an unusually large number of DGs are created for a fission or activation event. This warning has been added because a sparse amount of faulty data in cinder.dat will cause abnormally large numbers of DGs to be produced occasionally.

For 2.7.B, execution was halted and a message was posted if a fission or activation event resulted in more than a specified quantity, *nattm*, of decay products for a residual nuclide. For 2.7.D, the message has been changed to a warning. Execution continues with the number of nuclides in a decay limited to *nattm*. Thus, contributions to an event's CDF from nuclides further down the decay chain are omitted. Lengthy decay chains typically do not occur for fission events, but can occur for activation events when the activation involves uranic or transuranic nuclides.

MCNPX does not support the restart feature for delayed-particle calculations.

¹ J. W. Durkee, M. R. James, G. W. McKinney, H. R. Trelue, L. S. Waters, and W. B. Wilson, "Delayed-Gamma Signature Calculation for Neutron-Induced Fission and Activation Using MCNPX, Part I: Theory," *Progress in Nuclear Energy*, **51**, pp. 813–827 (2000)

3.23 UPDATED OUTPUT FILE FORMAT FOR PTRAC EVENT=CAP

Five additional columns of output information have been added to the `EVENT=CAP` option of the `PTRAC` card. The fifth column of output now provides the Z Aid identifier of the spontaneous fission nuclide. A value of 0 appears if the source is not spontaneous fission, i.e., `PAR=SF`. The sixth column contains the Z Aid of the first induced fission; the seventh, that of the second induced fission; the eighth, that of the third induced fission; and the ninth, that of the last fission before capture, either induced or spontaneous. If `DECN(23)>0`, only the four-column output, like that in v.2.7.B, is provided.

3.24 FULL ZAID IDENTIFIERS ON MX CARD

Full Z Aid identifiers are now supported on the `MX` card. This ability allows not only nuclide substitution, but also library substitution (e.g., the user may replace `ZZZAAA.60c` with `ZZZAAA.70c`).

Example:

```
m1      8016 1.0
        82206 10.0
        nlib=.60c
        hlib=.24h
        pnlib=.24u
mx1:h   j 26056.70h
mx1:n   j 88223.70c
mx1:p   j 94239.70u
```

MCNPX will use `8016.60c`, `8016.24h` and `8016.24u`. MCNPX will substitute `82206.60c` with `88223.70c`, `82206.24h` with `26056.70h` and `82206.24u` with `94239.70u`.

3.25 NESTED READ CARD

`READ` cards may now appear in auxiliary files. Nested `READ` cards are allowed and there is no limit on the number of nested levels. The encryption capability may be applied to any or all of the `READ` levels.

3.26 NCIA UPGRADE

MCNPX now can produce correlated secondary ions from neutron elastic and inelastic collisions. This capability is controlled by the seventh entry, `recl`, on the `PHYS:N` card.

The neutron capture ion algorithm (NCIA) in v.2.7.C is only activated if `recl>1` and there are no corresponding ion production data in the nuclear data table. In cases where correlated sampling is desired, it is necessary to have the NCIA active even when there are corresponding ion production data in the nuclear data table.

The NCIA option has been extended to allow correlated ion production.

As in previous versions of MCNPX,
if `recl=0`, then no light ion recoil occurs and no neutron capture ions are created.

In v.2.7.D,

$recl=n.m$, where m is a specified fractional value and n is an integer.

If $0 < m \leq 1$, and $n=0,1,2$, or 4 , then m is the number of light ions (protons, deuterons, tritons, ^3He , and alphas) per incident neutron to be created at each neutron elastic scatter event with light nuclei H, D, T, ^3He , and ^4He . Heavy ions are also created if they are a transported particle type (i.e., # appears on the MODE card).

If $n=3$ or $n=5$, then $m=0$ and light ion recoil is turned off.

For $n=2$ or $n=3$, the neutron capture ion algorithm (NCIA) is active when the NCIA reactions are not modeled with the nuclear data tables.

For $n=4$ or $n=5$, the neutron capture ion algorithm (NCIA) is active and the nuclear data tables for production of NCIA ions are deleted from the problem.

Light ion recoil (LIR) creates from $0 < recl < 1$ ions of type H, D, T, S, A, # when neutron or protons have elastic scatter with one of these nuclei.

The NCIA creates the correct number of secondary ions from neutron capture for certain important reactions. It may be used when these secondary particle production reactions are missing from the nuclear data tables or may be used to override the production in the nuclear data tables.

In summary,

if	$recl = 0$	Light ion recoil is off, NCIA is off (default)
if	$.001 < recl < 1.001$	Light ion recoil makes $recl$ ions from elastic scatter
if	$1.001 < recl < 2.001$	Light ion recoil makes $recl-1$ ions from elastic scatter; NCIA ions from neutron capture*
if	$recl = 3$	Light ion recoil is off, NCIA ions from neutron capture*
if	$3.001 < recl < 4.001$	Light ion recoil makes $recl-3$ ions from elastic scatter, NCIA ions from neutron capture [†]
if	$recl = 5$	Light ion recoil is off; NCIA ions from neutron capture [†]

* table data ion production will be used if possible

[†] NCIA will be used regardless if table data are available

3.27 M0 DEFAULT KEYWORD SPECIFICATION CARD

When the value of $m=0$ for the Mm material card, the M0 designation may be used to specify default cross-section libraries using the keywords NLIB, HLIB, PLIB, PNLIB, and ELIB. These library specifications (e.g., NLIB=.70c) will be applied to all Mm cards. Any library keyword value specified on an Mm card ($m \geq 1$) will override the default library specifications on the M0 card.

3.28 MINOR ENHANCEMENTS:

- $E > 1$ TeV/nucleon Warning: The warning for source particles with $E > 1$ TeV/nucleon was improved. Suggested by Robert Singleterry (NASA) (MRJ/GWM)
- Removed DBCN(20) which caused tracking with MCNPX 2.5.0 (JSH)
- Removed DBCN(21) which caused tracking with MCNPX 2.5.E (JSH)
- Removed DBCN(25) which turned off the Eric Pitcher / Bob Little $S(\alpha,\beta)$ broadening enhancement in MCNPX2.6.0 (JSH)
- Deleted the screen print of contour levels during geometry plots unless contour levels were set by the user. (JSH)
- The printout of perturbations of k_{eff} in criticality calculations (KCODE) now provides both the perturbation program and problem number. That is, if the 5th perturbation is PERT120:n, then both 5 and 120 are printed to identify the perturbation (as is done for tally perturbations) instead of just 5. Suggested by Jeff Favorite, LANL, X-1. (JSH)
- Some formats were expanded to print out as many as 999,999,999 histories. Suggested by Robert Singleterry, NASA. (GWM)
- Build system for MPI on Windows now expects to link to MPICH2 by default instead of MPICH1. (MRJ)
- WIN64 is now an accepted parameter for Windows configure script. This makes most, but not all, changes necessary for building on Windows 64-bit systems (XP/Vista/WIN7). (See Installation notes for Windows 64-bit builds available on the MCNPX web page.)
- It is now possible to build with the Intel 10 compiler with non-zero optimization on Linux and Windows. This is done by an automatic selective downgrading of the optimization in certain parts of the code.
- Beginning with Version 2.7.C, MCNPX offers improved support for Solaris operating systems.
- AIX/xlf is supported beginning in Version 2.7.C; however, the LLNL photofission multiplicity feature is not available for this system.
- Linux/gfortran is now supported for GNU/gcc versions 4.3 and above.

4 MCNPX CORRECTIONS

4.1 SIGNIFICANT PROBLEM CORRECTIONS

The following problems could cause incorrect answers. Fortunately, they occurred only in very special situations and affected only a few MCNPX users.

MCNPX v.2.7.A corrections to MCNPX v.2.6.0

4.1.1 Minor Burnup Reaction Rates Off

Data were loaded incorrectly (off by one energy bin) into the CINDER90 63-group flux bin structure for determining the contribution of a specific track traverse for a given burn material cell. The error only affected burnup/depletion for minor reactions that are treated with the 63-group fluxes—not fission, capture, or other major reactions that are treated continuously. The effect is generally so small as to be unnoticed in benchmark calculations. The error was a bug in

the binary search algorithm in the `burn_trk.F` subroutine and has been in all MCNPX versions with burnup. Non-burnup problems were unaffected. A \$20 award was made to Charles Whitmer (Whitmer Consulting, North Bend, WA) (X-3:08-77). (MLF)

4.1.2 Spontaneous Fission Normalization Error

When there is a spontaneous fission source ($PAR=SF$) and there is more than one spontaneous fission nuclide in a cell, then the relative weighting of source strengths was done based upon spontaneous fission yield data. However, MCNPX uses yield data in gram units and did not convert to atom units for the relative weighting. This error only affects spontaneous fission when there is more than one spontaneous fission nuclide in the cell. Whereas spontaneous fission is only done with actinides whose mass and atom fractions are similar, the effect is small and generally within the uncertainty of the yield. The error has been in MCNPX 2.6.0 and earlier versions. (MRJ)

4.1.3 DXTRAN Fail with Repeated Structures

Contributions from repeated structure/lattice cells to DXTRAN spheres are incorrect because the lattice level is not saved. This applies to all previous code versions including MCNPX 2.6.0 and MCNP5. There is no problem with only one DXTRAN sphere, but with additional DXTRAN spheres or point detectors, the lattice level index is wrong and particles can get lost, cause a crash, or cause silent wrong answers. A \$2 award was made to Richard Olsher, LANL RP-2 (X-3:JSH-09-007). (GWM)

4.1.4 Heavy Ion Errors

The heavy ion *ipt* is set to the ZA in bankit for banking heavy ions, but it was not being set back to *mipt*. This could lead to out-of-bounds array calls and other errors if the banking routine expected to use the *ipt* value after the bankit call. In bankit, the *ipt* is now restored to *mipt* after a heavy ion is banked. (MRJ)

4.1.5 $S(\alpha,\beta)$ File Reading Failure

If $S(\alpha,\beta)$ data files are mixed in with other types of data files (like neutron or photon data tables) and if they are read before the other tables, some cross-section pointers can be incorrect causing wrong answers. The problem affects MCNPX 2.6.0 and all previous versions. In one case, k_{eff} was wrong by a factor of two. Note that none of the data libraries distributed with MCNP/MCNPX mixes $S(\alpha,\beta)$ and other data table types. Therefore, this is only a problem for users who mix data type when constructing their own libraries of nuclear data tables. (GWM)

4.1.6 Burnup Continue Runs

Continue runs of burnup problems that included the `MATVOL` or `MATMOD` keywords did not track and were wrong because arrays *bvol* and *conb* were not written to the RUNTPE file. These arrays are now written to the RUNTPE file and continue runs now work with all burnup capabilities. (MLF)

MCNPX v.2.7.B corrections to MCNPX v.2.7.A

4.1.7 Heavy Ions

Heavy ions put in the bank for subsequent transport within a given history came out of the bank with a particle number equal to the heavy ion Z Aid rather than the heavy ion particle type. Thus

lithium-6 going into the bank with `ipt=35` (particle type for heavy ions, `par=#`) would come out of the bank with `ipt=3006`. The error could cause an array overflow with unpredictable consequences. In most cases charged particles and heavy ions bank all their progeny and then retrieve the heavy ions from the bank so this would be no problem. The error did not touch any of the MCNPX extended test set heavy ion problems. However, in one case it caused the heavy ion model physics for transport of 3006 to terminate with “distance to event = zero” because the time cutoff was overwritten. The error has been present for all versions with heavy ion transport and affects only heavy ions. A \$20 award was made to Uwe Titt, University of Texas M. D. Anderson Cancer Center, Houston, Texas, X-3:09-016 (JSH)

4.1.8 Spontaneous Fission Automatic Weighting

The automatic weighting of spontaneous fission (`SPn w` option) gave incorrect source neutron weights because the gram density rather than the atom density was used in the calculation. Consequently the calculation of maximum source weight was incorrect and the minimum source weight calculation has not yet been extended to the `SPn w` option. Finally, the use of non-unity weights in the `FT8 CAP` capture tally option caused by the automatic weight option was not anticipated; consequently the relative error in the moments calculation has been extended to accommodate source weights not equal to one. A \$20 award was made to Martyn Swinhoe, LANL N-1, X-3:09-017 (MRJ/JSH)

4.1.9 Spontaneous Photon Material/Cell Error

With multiple materials and cells, the `SP` source would get confused and report that no radioactive nuclides were found. The `act()` array was found to have used an incorrect index in the `spn_phot` routine. (MRJ)

MCNPX v.2.7.C corrections to MCNPX v.2.7.B

4.1.10 Photonuclear Delayed Neutrons

The `nter` variable was not being properly set for photonuclear delayed particles causing the secondaries not to be banked. A \$20 award was made to John Apruzese, Naval Research Laboratory, D-5:09-049. (GWM)

4.1.11 Type 2 (Source) Mesh Tally

The source mesh tally previously recorded all bank events as “source” particles, including variance reduction events such as splitting. The `mspf` variable has been updated so that all bank events set `mspf` correctly and variance reduction bank events are ignored. A \$2 Award was made to Timco Visser, URENCO Nederland BV, D-5:09-048. (MRJ)

4.1.12 Isomer Specifications with Model Physics

Isotopes specified with the new isomer convention (`A+300+100*state`) would fail with models because the `A` value (i.e., atomic mass) was out of range. A correction was added to give the ground-state `A` value for these cases. A €20 note was awarded to Carlo Petrovich of ENEA FIS-NUC Bologna, Italy, D-5:09-050. (MLF)

4.1.13 Shared RUNTPE Rendezvous

Rendezvous frequency was being improperly set for some runs when RUNTPE sharing was turned on. A \$20 award was made to Edward Siciliano, Pacific Northwest National Laboratory, D5:10-002. (GWM)

4.1.14 Type 3 Tally Tag

Tagging was corrected for elastic scatter in libraries and models. A \$20 award was made to Steve Swanekamp, L-3 Communications, D5:10-003. (MRJ)

*MCNPX v.2.7.D corrections to MCNPX v.2.7.C***4.1.15 LAQGSM Initialization**

The random numbers generated by LAQGSM in initialization are now done internal to the model. This restores tracking for continue-runs with LAQGSM. (GWM)

4.1.16 Special Tally Treatment FT PHL with Source Biasing

The pulse-height light tally special treatment (FT8 PHL) would give different answers when source biasing was used. The FT8 PHL tally was incorrect when dose functions (DE_n, DF_n) were not used and when source weights were not equal to one. Note that it has always been a warning error to not have dose functions with the FT8 PHL treatment. Further, source weights are equal to one except in the cases of (1) specification of non-unit weight, such as SDEF WGT=*nnn*; (2) source biasing with an SB card; or (3) variance reduction, which is a fatal error for FT8 PHL. MCNPX has been corrected so that FT8 PHL now works if SDEF WGT=*nnn* or SB_n are used. A \$20 award will be made to Michael King, Rapiscan Laboratories. (MRJ)

4.1.17 SP Normalization

SP source normalization used incorrect time value for integration in dng_model. A \$20 award was made to Edouard Malambu, SCK•CEN, D5-10-042. (MRJ)

4.1.18 BURN Card (n,γ) Cross Section

The (n,γ) reactions rates being reported to CINDER90 were actually total absorption rates. To accelerate the computation of (n,γ) reaction rates, total absorption was used as an approximation for (n,γ). For many nuclides, total absorption is roughly equal to (n,γ); however, in some light ions, such as ¹⁰B, (n,α) dominates capture, and therefore total absorption is not roughly equal to (n,γ). MCNPX now calculates the actual (n,γ) contribution. A \$20 award was made to George Zimmerman (D5:010-041). (MLF)

4.1.19 BURN Card MAT/MATVOL Reorder

When using a MATVOL keyword, if material card numbers on the MAT keyword of the BURN card were not listed in ascending order, MCNPX would accidentally reorder these volumes using integer representation of a floating point number. This issue has been fixed. A \$20 award was made to Al Hanson, Brookhaven National Laboratory, D5:010-048 (MLF)

4.2 MINOR PROBLEM CORRECTIONS

The following problems do not cause wrong answers, but they may cause crashes when encountered. In any case, they occurred only in very special situations and affected only a few MCNPX users.

MCNPX v. 2.6.0 corrections to MCNPX v.2.6.F

4.2.1 INTEL Compiler Workaround

Large problems failed with the INTEL 10 compiler requiring a workaround. A \$2 award was made to Manuel Bardies (INSERM, Nantes, France) (X-3:JSH-2008-050). (GWM)

4.2.2 LAQGSM Corrections

LAQGSM Standalone: The LAQGSM module compiled as a standalone code wrote to the wrong unit number. (GWM)

LAQGSM Infinite Loops: Several instances of infinite loops in LAQGSM have been identified and are now resampled to prevent MCNPX from hanging. (MRJ)

Coulomb Barrier Physics: Coulomb barrier physics has been added for heavy ions. (MRJ)

Heavy Ion SPABI: Secondary particle production biasing, the SPABI input card option, failed for heavy ions and has been corrected. (MRJ)

4.2.3 Compiler Workaround

The floating point variable TDS was used in a ‘do loop’ in routine ITALLY. (This is a harmless error or compile error, depending upon the system.) An award of €20 was made to Frank Gunsing, (CEA/Saclay, France) (X-3:JSH-2008-045). (JSH)

4.2.4 Detector Tallies in Lattice Geometries

If a detector tally contribution is from a cell filled with a lattice, then the mesh type 4 or point detector tallies did not score. A \$2 award was made to Róbert Kákonyi (University of Szeged, Hungary) (X-3:JSH-2008-049). (GWM)

MCNPX v.2.7.A corrections to MCNPX v.2.6.0

4.2.5 Burnup Duplicate ZAIDs

Duplicate ZAIDs on a materials card caused burnup to crash. A \$20 award was made to Gregory A. Johnson (Hamilton Sunstrand–Rocketdyne, Canoga Park, CA) (X-3:08-60). (MLF)

4.2.6 Source Particle Types Unrecognized in Dependent Distributions

Specification of different source particles in dependent distributions is unrecognized. For example, the combination

```
SDEF PAR=FPOS=D99
```

and

```
DS99 S D12 D13
```

fails and gives spurious warning messages. MCNPX thinks D12 and D13 are particle types rather than distributions (where the particle types would then be specified). An award of \$20 was made to Gregory Thoreson (LANL D-5) (X-3:08-78). (LSW/JSH)

4.2.7 Incorrect Warning Error for Detector Tallies

The error message “tally not scored beyond last time bin” for detector tallies printed the time at the collision rather than the time at the detector for point/ring detectors. The bug was in all previous MCNP, MCNP5, and MCNPX versions. A \$2 award was made to Bill Sailor (LANL, ISR-4) (X-3:08-76). (GWM)

4.2.8 Choice of High-Energy Mode

Neutrons, protons, or deuterium colliding with neutrons, protons, or deuterium at high energies should go to FLUKA, not LAQGSM. A \$2 award was made to Sukesh Aghara (Prairie View A&M University, Texas) (X-3:JSH-2008-048). (MRJ)

4.2.9 Lost Particles Cause Crash

See Section 4.1.3 – DXTRAN fails with repeated structures.

MCNPX v.2.7.B corrections to MCNPX v.2.7.A

4.2.10 Tally Tagging Labels

Tally tagging labels were inconsistent for reactions from physics models and data tables. Also, the fatal error for tagging not working for anything but neutrons and photons was removed. (GWM)

4.2.11 Heavy Ion Direction Cosines

CEM velocity vectors rather than direction cosines for outgoing residual nuclei were being passed to MCNPX. The resulting incorrect direction cosines resulted in heavy ion transport errors, infinite loops, or crashes. A \$2 award was made to Richard Olsher, LANL RP-2, X-3:09-019 (MRJ/JSH)

4.2.12 Cylindrical Mesh Tally

Particles transporting exactly on the axis of a cylindrical mesh tally would not score in any bin. The code now scores the flux correctly but only in the case when one theta bin is specified. Use of multiple theta bins in this case is a fatal error. (MRJ/JSH)

4.2.13 Stopping Power Bin Control

The stopping power bin control, the 11th entry on the PHYS:<p1> card, where <p1> is any charged particle type, was documented for 2.7.A but was not actually present. This feature is now implemented. (JSH)

4.2.14 Revised GDR.DAT

The gdr.dat file was updated and the new version is being distributed with the code. The only change is a correction to the krypton isotopes. (MRJ)

4.2.15 Muon Physics

Timing delays for muon capture were added based in Primakov probabilities. K-L x-ray line emissions were corrected (energies values were swapped in previous versions). Muon capture physics is now turned on for all isotopes, not just those with x-ray line information. (MRJ)

4.2.16 Light Ion Production from Inelastic Collisions

The B-10 capture reaction now emits Li-7 as a heavy ion and the Q-value was changed to the correct value of 2.79 MeV. (MRJ)

4.2.17 Isomer Branching in Burnup

The $M(n, g)N$ reaction rate sent to CINDER90 is now adjusted to use the true yield adjust (n, g) reaction rate instead of $M(n, g)N^* + M(n, g)N$ sent in the previous version. The yield adjusted $M(n, g)N$ reaction rate is determined by using the ratio of the $M(n, g)N^*$ cross section calculated by CINDER90 and the $M(n, g)N^* + M(n, g)N$ cross section calculated by MCNPX as shown in the following equation: (MLF)

$$\text{corrected } M(n, g)N = \left\{ 1 - \frac{M(n, g)N^*_{CINDER90}}{[M(n, g)N^* + M(n, g)N]_{MCNPX}} \right\} \times [M(n, g)N^* + M(n, g)N]_{MCNPX}$$

4.2.18 PTRAC Capture Events

If user specifies `EVENT=CAP` on the PTRAC card, and if the user specifies `MAX<0`, then the run will cease after `|MAX|` PTRAC captures have occurred. (MLF)

4.2.19 Burnup Tier 3 Fission Products

Because of the lack of ENDF VII.0 transport cross-section data, the following nuclides have been eliminated from the Tier 3 burnup fission product generator list: 39088, 41097, 53132, 53133, 53134, 59145, and 69169. (MLF)

4.2.20 KCODE Fission Source in MPI

If the user quits a KCODE run during a parallel operation, the fission source is collected to be saved on the RUNTPE file for continue runs. (MLF)

During parallel execution of KCODE, if a processor does not generate any new source particles for a given cycle, the fission source is collected and redistributed. (MLF)

4.2.21 CEM/LAQGSM

CEM now initializes when muons are on the `MODE` card. (MRJ)

Several CEM/LAQGSM bugs were fixed. (SGM/REP)

Incorrect initialization in LAQGSM caused the code to fail on Sun machines. A \$2 award was made to Kyle Copeland, D-5:09-032. (MRJ)

4.2.22 Delayed Neutron / Delayed Gamma Correction

Subroutine `rotas` calls in delayed neutron/delayed gamma problems were corrected; the calls improperly used parameter `uold` as a vector. In rare cases, this improper use caused incorrect

azimuthal angles after scattering resulting in incorrect direction cosines. Found by Tom Miller. (MRJ)

4.2.23 Secondary Particle Arrays Increased

To avoid heavy ion and delayed neutron/delayed gamma array overflows, the l02, l05 parameters for secondary particle arrays were increased to 2500 from 2000. (MRJ)

4.2.24 MPI Run Wall Clock Correction

Timing bug fixed in C code. An incorrect multiplier that was introduced in 2.7.A to the millisecond field caused random wall clock times in MPI parallel runs. Also applied at this time was a fix to the resolution of timing calls, which were improved from 128 seconds to milliseconds. Reported by Dudley Raine, to whom \$20 was awarded, D-5:09-034 (MRJ)

4.2.25 Uninitialized or Out-of-Bounds Arrays

A number of uninitialized variables and out-of-bounds arrays were found in the MCNP6 / MCNPX merged version and corrected in MCNPX 27B. (JSH/MRJ)

MCNPX v.2.7.C corrections to MCNPX v.2.7.B

4.2.26 Intel 11.0 Compatibility

Source subroutines were updated to permit compiling with Intel v11.0. (JWD/JSE)

4.2.27 Table 38 Printing

Table 38 is now controlled by the correct option on the PRINT card. Reported by Victor Gavron, to whom \$20 was awarded, D-5: 09-047. (MRJ)

4.2.28 Interactive Plotting Commands

Commands issued during interactive plotting are now recorded in a COMOUT file. (MRJ)

4.2.29 Spontaneous Photon Zero-Volume Cells

An error trap has been added to catch when SP W option is used with a zero-volume cell. (MRJ)

4.2.30 TIR/TIC Bug Fix

When the radiography grid was centered on the origin (0,0,0), the origin could not be used to locate the center of a TIR/TIC radiography tally. A different approach is now invoked when the grid is centered on the origin to avoid this problem. (GWM)

4.2.31 Tally Multiplier (FM) Cards with Mesh Tallies

Tally multiplier (FM) cards with mesh tallies previously required a dummy tally to prevent expunging data and could not be used with a dummy (unused) material. Both have been corrected. An award of \$2 was made to Jianwei Hu (LANL, N-4) (D-5:09-52). (MLF)

4.2.32 Burnup Corrections Regarding Fission Energy Boundaries

The energy threshold that distinguishes between fast and thermal fission spectra was adjusted. The following three energy regimes were defined. 1) thermal, less than or equal to 1 eV; 2) fast, greater than 1 eV and less than or equal to 14 MeV; and 3) high energy, greater than 14 MeV. (MLF)

4.2.33 Torus Major/Minor Axes Ratio

Tracking errors could occur when the ratio of a torus' major to minor axes exceeded $2e4$. A warning will be printed for these cases. (JWD) Volume calculations for tori with large aspect ratios also can be incorrect, causing improperly normalized flux tallies in these regions.

4.2.34 CEM Upgrades

Various minor upgrades and corrections were applied to CEM 3.02. (SRM)

4.2.35 INCL Bug Fixes

Various minor corrections were made to the INCL/ABLA package. (REP)

4.2.36 IC=-99 Units Correction

The implementation of the dose multiplier did not report the results directly in SI units. A multiplier is now used to make the units consistent with other tally options. (GWM)

4.2.37 Burnup Correction Sending Isomer Reaction Rates to CINDER90

Previously, reaction rates for metastable isotopes were not accepted by CINDER90 regardless whether they were calculated by MCNPX. This issue is now fixed. (MLF)

4.2.38 Using a PHYS:N Card with Burnup

The first entry on the PHYS:N card can now exceed the maximum energy of the tabular cross section when using a BURN card. A \$20 award was made to Anthony Scopatz (University of Texas-Austin), D-5:09-051. (MLF)

4.2.39 Burnup MODE N P

A bug existed that caused the neutron interaction rates to be updated using photon transport track lengths leading to anomalous answers in MODE N P calculations with a BURN card. A \$20 award was made to Kenneth S. Allen (University of South Carolina), D-5:10-001. (MLF)

*MCNPX v.2.7.D corrections to MCNPX v.2.7.C***4.2.40 GBR Fix**

Gaussian energy broadening was corrected to prevent the possible creation of negative energies by the broadening adjustment. (MRJ)

4.2.41 Cinder Compatibility with FORTRAN Compilers

The Cinder code module was fixed to allow compilation with the gfortran and g95 compilers. (MRJ)

4.2.42 Recoil with Heavy Ions

The warning message for elastic recoils was corrected so that it now checks for heavy ions on the MODE card. (MRJ)

4.2.43 SETRES Bug Fix

The setres.F routine would try to produce a residual from reactions that occurred in elemental libraries and produce an invalid isotope. The routine was fixed to sample from natural isotopic distribution. (MRJ)

4.2.44 MSCAT Bug Fix

The MSCAT3 routine relied upon variables in LCS routines that might not be set before its first call. The routine was changed to use variables declared in the GLOBAL modules. (MRJ)

5 FUTURE WORK

The following projects are at least partially funded and are actively being developed:

- Additional CINDER90 capabilities:
 - Burnup / depletion enhancements;
 - Fixed source depletion;
 - Automatic production of background activation; and
 - Automatic production of radioactive sources;
- Correlated secondary particle production;
- Automatic natural background sources;
- Aged spontaneous photon sources;
- Extending photon and electron physics down to 1 eV;
- Adding Cerenkov, synchrotron, transition radiation physics;
- Standard optical photon physics (i.e., reflection, refraction);
- Delta rays for all charged particles;
- Moving objects;
- Allowing multiple keywords on FT8 cards;
- Addition of light-ion libraries;
- Delayed betas and alphas;
- Improvements in photonuclear cross sections and yields; and
- INCL upgrade to the latest version.

The following projects are on our wish list. Some have been partially developed but await further funding.

- Improved convergence of eigenfunctions in criticality problems;
- Integration of HTAPE tallies directly into MCNPX, including continue runs;
- Electric and magnetic field tracking;
- Detectors and DXTRAN for all neutral particles at all energy ranges with anisotropic scattering (currently approximated as isotropic for models);
- CAD link;
- Secondary particle angle biasing for isotropic distributions;
- Neutral particle perturbation techniques extended to physics model region;
- Plotting of physics model total and absorption cross sections; and
- Forced collisions for neutral particles extended to physics models.

APPENDIX A

APPENDIX A: IMPROVEMENT OF DNDG EMISSION-SPECTRA ACCURACY

In versions of the MCNPX code prior to v. 2.7.D, DNDG calculations used the trapezoidal rule numerical algorithm to perform the CDF time-integration.[†] In version 2.7.D, this algorithm has been replaced by analytic evaluation for a residual nuclide.

A.1 CDF FORMULATION

The time- and energy-dependent source of delayed particles is created by the decay of all fission products and their daughter products. The source contribution for the \tilde{i}^{th} fission-product of interest, $\text{FP}_{\tilde{i}}$, and its decay products for each $\tilde{i} - N_{\tilde{i}}$ total nuclides—can be written as

$$s_{\tilde{i}\tilde{n}}^L(E, t) = N_{\tilde{i}\tilde{n}}(t) \lambda_{\tilde{i}\tilde{n}} p_{\tilde{i}\tilde{n}}^L(E) \quad (\text{gammas/m}^3\text{-s-MeV}), \quad (1)$$

where $s_{\tilde{i}\tilde{n}}^L(E, t)$ is the energy- and time-dependent number of delayed particles produced by nuclide \tilde{n} , $N_{\tilde{i}\tilde{n}}(t)$ is the time-dependent nuclide atom density for the \tilde{n}^{th} radioactive decay species associated with the \tilde{i}^{th} fission product (atoms/m^3), $\lambda_{\tilde{i}\tilde{n}}$ is decay constant for $\text{FP}_{\tilde{i}}$ and nuclide \tilde{n} (s^{-1}), and $p_{\tilde{i}\tilde{n}}^L(E)$ is the delayed-gamma production probability at energy E for $\text{FP}_{\tilde{i}}$ and nuclide \tilde{n} (gammas/MeV-atom).

Integration of Eq. (1) over all energy and time gives the total number of delayed gammas emitted per fission or activation event for \tilde{i} and \tilde{n} due to line emission:

$$S_{\tilde{i}\tilde{n}}^L = \int_0^\infty \int_0^\infty s_{\tilde{i}\tilde{n}}^L(E, t) dE dt \quad (\text{gammas/m}^3). \quad (2)$$

The line data are represented as a series of values at discrete energies. Thus, the line sources are conveniently represented using Kronecker delta functions so that

$$p_{\tilde{i}\tilde{n}}^L(E) = \sum_{k=1}^{\tilde{K}} \delta(E_k) p_{\tilde{i}\tilde{n}}^G(E) \quad (\text{gammas/MeV-atom}), \quad (3)$$

where the Kronecker delta function is

$$\delta_k = \begin{cases} 0 & \text{for } E \neq E_k \\ 1 & \text{for } E = E_k \end{cases}, \quad (4)$$

$p_{\tilde{i}\tilde{n}}^G(E)$ is the general nuclide emission function, and \tilde{K} is the total number of lines.

[†] Durkee J.W., Jr., James M.R., McKinney G.W., Trelue H.R., Waters L.S., and Wilson W.B. (2009), “Delayed-Gamma Signature Calculation for Neutron-Induced Fission and Activation Using MCNPX, Part I: Theory,” *Progress in Nuclear Energy*, 51, 813–827.

Recall that the cindergl.dat data also include so-called continuous contributions for many nuclides. The continuous data are differential data; thus, they are integrated (over their 10-keV bin structure) before being used with the discrete-emission data.

By inserting Eq. (3) into Eq. (1), substituting the result of Eq. (1) into Eq. (2), and integrating over energy, we get

$$\begin{aligned} S_{\bar{i},\bar{n}}^L &= \int_0^\infty N_{\bar{i},\bar{n}}(t) \lambda_{\bar{i},\bar{n}} \sum_{k=1}^{\bar{K}} p_{\bar{i},\bar{k},\bar{n}}^L dt \\ &= \int_0^\infty \sum_{k=1}^{\bar{K}} N_{\bar{i},\bar{n}}(t) \lambda_{\bar{i},\bar{n}} p_{\bar{i},\bar{k},\bar{n}}^L dt \quad (\text{gammas/m}^3), \end{aligned} \quad (5)$$

where

$$p_{\bar{i},\bar{k},\bar{n}}^L = p_{\bar{i},\bar{n}}^G(E_{\bar{k}}). \quad (6)$$

The total DG source is obtained by summing $S_{\bar{i},\bar{n}}^L$ over all fission products (or residual nuclides) for a fission (or activation) event and all of the decay products so that

$$S^L = \sum_{\bar{i}=1}^{\bar{I}} \sum_{\bar{n}=1}^{\bar{N}\bar{i}} \int_0^\infty \int_0^\infty s_{\bar{i},\bar{n}}^L(E,t) dE dt. \quad (7)$$

The general expression for S^L is not available in analytic form because of the complexity of $N_{\bar{i},\bar{n}}(t)$ that is embedded in $s_{\bar{i},\bar{n}}^L(E,t)$. Thus, the integral expressions in Eq. (7) must be evaluated approximately. To do so, the integrand in Eq. (7) is written in the approximate finite-limit form

$$S_{\bar{i},\bar{n}}^L \approx \sum_{j=1}^J \sum_{k=1}^{\bar{K}} \int_{t_{j-1}}^{t_j} \int_{E_{k-1}}^{E_{\bar{k}}} s_{\bar{i},\bar{n}}^L(E,t) dE dt \quad (\text{gammas/m}^3). \quad (8)$$

Until version 2.7.D of MCNPX, the integral in Eq. (8) was evaluated using the trapezoidal rule:

$$\bar{N}_{\bar{i},\bar{j},\bar{n}} = \frac{\int_{t_{j-1}}^{t_j} N_{\bar{i},\bar{n}}(t) dt}{\int_{t_{j-1}}^{t_j} dt} \approx \frac{\int_{t_{j-1}}^{t_j} (N_{\bar{i},\bar{j}-1,\bar{n}} + m_{\bar{i},\bar{j},\bar{n}} t) dt}{\Delta t_j} = \frac{N_{\bar{i},\bar{j}-1,\bar{n}} + N_{\bar{i},\bar{j},\bar{n}}}{2} \quad (\text{atoms/m}^3), \quad (9)$$

where

$$\Delta t_j = \int_{t_{j-1}}^{t_j} dt \quad (\text{s}), \quad (10)$$

and

$$m_{\bar{i},\bar{j},\bar{n}} = \frac{N_{\bar{i},\bar{j},\bar{n}} - N_{\bar{i},\bar{j}-1,\bar{n}}}{\Delta t_j}. \quad (11)$$

Incorporating the results of Eqs. (9)–(11) leads to

$$S_{\tilde{i}:J,\tilde{k},\tilde{n}}^L = \sum_{j=1}^J \sum_{\tilde{k}=1}^{\tilde{K}} \bar{N}_{\tilde{i}:j,\tilde{n}} \Delta t_j \lambda_{\tilde{i},\tilde{n}} p_{\tilde{i}:\tilde{k},\tilde{n}}^L \quad (\text{gammas/m}^3). \quad (12)$$

Then, using Eq. (9), the summand in Eq. (12) can be rewritten as

$$S_{\tilde{i}:j,\tilde{k},\tilde{n}}^L = \left[\frac{(N_{\tilde{i}:j-1,\tilde{n}} + N_{\tilde{i}:j,\tilde{n}}) \Delta t_j}{2} \right] \lambda_{\tilde{i},\tilde{n}} p_{\tilde{i}:\tilde{k},\tilde{n}}^L \quad (\text{gammas/m}^3). \quad (13)$$

A.2 ANALYTIC INTEGRATION

In version 2.7.D of MCNPX, evaluation of the time integral in Eq. (8) has been improved using an analytic integration scheme.

For a residual nuclide, the atom density is given by the simple expression

$$N_{\tilde{i}:1}(t) = N_{\tilde{i}:0,1} e^{-\lambda_{\tilde{i}} t} \quad (14)$$

so that the integral in Eq. (5) evaluates to

$$S_{\tilde{i}:J,\tilde{k},1}^L = \sum_{j=1}^J \sum_{\tilde{k}=1}^{\tilde{K}_{11}} N_{\tilde{i}:0,1} \left(e^{-\lambda_{\tilde{i}} t_{j-1}} - e^{-\lambda_{\tilde{i}} t_j} \right) p_{\tilde{i}:\tilde{k},1}^L, \quad (15)$$

where $N_{\tilde{i}:0,1}$ is the atom density of the principal nuclide ($\tilde{n} = 1$) at time zero, $N_{\tilde{i}:j}(t) = N_{\tilde{i}:0,j}$, $\tilde{j} = 1$. MCNPX DG calculations are done with the atom densities of the principal nuclides (fission and activation products) normalized to 1, i.e., $N_{\tilde{i}:0,1} = 1$.

MCNPX has been upgraded to calculate the time-dependent atom density of a residual nuclide using the analytic results in Eqs. (14) and (15). This upgrade pertains to residual nuclides that have stable daughters.

As an example, consider the two prominent emission lines for ^{60}Co at 1.1732 and 1.3325 MeV. From the cindergl.dat file, $p_1=0.999$ and $p_2=0.9998$. Analytic evaluation of the integral in Eq. (5) from time 0 to infinity as given by Eq. (15) with $N_{\tilde{i}:0,1} = 1$, $J = 1$, $\tilde{K}_{11} = 2$, $t_0 = 0$, and $t_1 = \infty$ gives an aggregate emission of $p_1+p_2=1.9988$ gammas/decay. Previous versions of MCNPX calculated an aggregate emission of 2.3855 γ /decay. MCNPX version 2.7.D calculates 1.9988 γ /decay.

The analytic evaluation of the atom density is available only for line-mode execution (ACT DG=LINES). For multigroup mode execution (ACT DG=MG), numerical evaluation is done.

A.3 DISCONTINUATION OF PREVIOUS NORMALIZATION PROCEDURE

In code versions previous to version 2.7.D, the line-emission data were multiplied by the ebf6 normalization factor contained in the cinder.dat file. By applying this factor, the summed line emission (in cindergl.dat) in a multigroup energy bin equated to its multigroup counterpart (in cinder.dat). This practice was satisfactory in ensuring that the integral multigroup and line

emission equated. Therefore, version 2.7.D discontinues the renormalization of DG line-emission data using the ebf6 factor.