

LA-UR-11-01502

*Approved for public release;  
distribution is unlimited.*

*Title:* MCNPX 2.7.E Extensions

*Authors:* Denise B. Pelowitz  
Joe W. Durkee  
Jay S. Elson  
Michael L. Fensin  
John S. Hendricks  
Michael R. James  
Russell C. Johns  
Gregg W. McKinney  
Stepan G. Mashnik  
Jerome M. Verbeke  
Laurie S. Waters  
Trevor A. Wilcox

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



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.



**MCNPX 2.7.E Extensions**

by

Denise B. Pelowitz  
Joe W. Durkee  
Jay S. Elson  
Michael L. Fensin  
Michael R. James  
Russell C. Johns  
Gregg W. McKinney  
Stepan G. Mashnik  
Laurie S. Waters  
Trevor A. Wilcox

Los Alamos National Laboratory

John S. Hendricks  
TechSource, Inc.

Jerome M. Verbeke  
Lawrence Livermore National Laboratory

March 2011

Copyright. Los Alamos National Security, LLC. All rights reserved.

This material was produced under U.S. Government contract DE-AC52-06NA25396 for Los Alamos National Laboratory, which is operated by Los Alamos National Security, LLC for the U.S. Department of Energy. The Government is granted for itself and others acting on its behalf a paid-up, nonexclusive, irrevocable worldwide license in this material to reproduce, prepare derivative works, and perform publicly and display publicly. Beginning five (5) years after (insert date permission to assert copyright was obtained), subject to additional five-year worldwide renewals, the Government is granted for itself and others acting on its behalf a paid-up, nonexclusive, irrevocable worldwide license in this material to reproduce, prepare derivative works, distribute copies to the public, perform publicly and display publicly, and to permit others to do so.

NEITHER THE UNITED STATES NOR THE UNITED STATES DEPARTMENT OF ENERGY, NOR LOS ALAMOS NATIONAL SECURITY, LLC, NOR ANY OF THEIR EMPLOYEES, MAKES ANY WARRANTY, EXPRESS OR IMPLIED, OR ASSUMES ANY LEGAL LIABILITY OR RESPONSIBILITY FOR THE ACCURACY, COMPLETENESS, OR USEFULNESS OF ANY INFORMATION, APPARATUS, PRODUCT, OR PROCESS DISCLOSED, OR REPRESENTS THAT ITS USE WOULD NOT INFRINGE PRIVATELY OWNED RIGHTS.

## TABLE OF CONTENTS

<b>1</b>	<b>INTRODUCTION .....</b>	<b>1</b>
1.1	Summary of New MCNPX Features .....	1
1.2	Availability .....	2
1.3	Documentation .....	2
1.4	Cash Awards Quality Assurance Program .....	2
<b>2</b>	<b>DESCRIPTION OF NEW MCNPX FEATURES .....</b>	<b>3</b>
2.1	Tally Tagging .....	3
2.1.1	User Interface .....	3
2.1.2	Usage and Special Cases .....	4
2.1.3	Examples .....	5
2.2	CEM 3.02 Upgrade .....	7
2.3	MCNPLOT Graphics and "HELP" Command Upgrades .....	9
2.3.1	Graphics Upgrades .....	9
2.3.2	"HELP" Command Upgrade .....	12
2.4	Embedded Sources .....	13
2.4.1	User Interface .....	13
2.4.2	Examples .....	14
2.5	Stopping Power Energy Table Control .....	17
2.6	Cyclic Time Bins .....	17
2.7	Focused Beam Source Option .....	18
2.7.1	User Interface .....	18
2.7.2	Example of Focused Beam Source .....	19
2.8	PTRAC Coincidence Option .....	22
2.9	LLNL Multiplicity .....	23
2.9.1	LLNL Photofission Multiplicities .....	23
2.9.2	LLNL Neutron Fission Multiplicities .....	24
2.10	Arithmetic MCNPLOT Options .....	27
2.10.1	Description .....	27
2.10.2	User Interface .....	27
2.10.3	Usage and Special Cases .....	28
2.10.4	Examples .....	29
2.11	Receiver-Operator Characterization (ROC) Tally Option .....	32
2.12	Pulse-Height Light Tally: Triple and Quadruple Coincidences .....	33
2.13	Time-Dependent F8 Tallies Using Pulse-Height Light Option .....	34
2.14	LAQGS 3.03 Upgrade .....	35
<b>3</b>	<b>MCNPX 2.7.E FEATURE EXTENSIONS AND ENHANCEMENTS .....</b>	<b>36</b>
3.1	Spontaneous Photon Features .....	37
3.1.1	Spontaneous Material Source .....	37
3.1.2	Spontaneous Gamma Particle Specification .....	37

3.1.3	Features and Defaults .....	37
3.1.4	Exponential Decay Function .....	38
3.1.5	SPn w Source Probability Option – Automatic Source Weight Adjustment .....	38
3.2	Burnup Enhancements .....	39
3.2.1	Parallelizing the CINDER90 Interface .....	39
3.2.2	Variable Dimensioning for Burnup and Spontaneous Photons .....	40
3.2.3	Unlimited MATMOD Changes .....	40
3.3	Lattice FILL Error Trap .....	40
3.4	Windows 64-bit Support/Compilation without Graphics .....	40
3.5	Special Treatment Tally for Electron Current .....	41
3.6	RUNTPE Initialization During MPI .....	41
3.7	New Special Treatment Tally: LET .....	41
3.8	ICRP-60 Dose Function .....	41
3.9	Residual Tally Upgrades .....	42
3.10	Lattice Cell Rejection for Sources .....	43
3.11	ACT: Activation Control Card .....	43
3.12	Replacement of <sup>235</sup> U Delayed Neutron Spectrum .....	44
3.13	Tally Fluctuation (TF) Card Extension for ROC Special Tally .....	44
3.14	FM Card Extension .....	45
3.15	Geometry Plotter: Contour Legend Addition .....	45
3.16	Expansion of Muonic X-Ray Database .....	45
3.17	Heavy-Ion Recoil .....	45
3.18	Exact Energy Integration Improves Delayed Gamma Spectra .....	46
3.19	Delayed Neutron/Delayed Gamma Calculations Using Implicit Capture .....	48
3.20	New Photoatomic Form Factors .....	49
3.21	Memory Reduction Options and Bank Size Control for MODE N P E Calculations .....	49
3.22	DNDG Speedup, Accuracy Improvement, and User Control .....	50
3.22.1	Delayed Gamma Execution-Time Reduction .....	50
3.22.2	Improvement in Delayed Neutron/Delayed Gamma Emission- Spectra Accuracy .....	51
3.22.3	Warnings and Notations Regarding DNDG Emissions .....	51
3.23	Updated Output File Format for PTRAC EVENT=CAP .....	51
3.24	Full ZAID Identifiers on MX Card .....	51
3.25	Nested READ Card .....	52
3.26	NCIA Upgrade .....	52
3.27	M0 Default Keyword Specification Card .....	53
3.28	New cinder.dat .....	53
3.29	Minor Enhancements: .....	55
<b>4</b>	<b>MCNPX CORRECTIONS .....</b>	<b>56</b>
4.1	Significant Problem Corrections .....	56

4.1.1	Minor Burnup Reaction Rates Off.....	56
4.1.2	Spontaneous Fission Normalization Error .....	56
4.1.3	DXTRAN Fail with Repeated Structures .....	56
4.1.4	Heavy Ion Errors .....	56
4.1.5	S( $a,\beta$ ) File Reading Failure.....	56
4.1.6	Burnup Continue Runs.....	57
4.1.7	Heavy Ions.....	57
4.1.8	Spontaneous Fission Automatic Weighting .....	57
4.1.9	Spontaneous Photon Material/Cell Error.....	57
4.1.10	Photonuclear Delayed Neutrons .....	57
4.1.11	Type 2 (Source) Mesh Tally.....	58
4.1.12	Isomer Specifications with Model Physics.....	58
4.1.13	Shared RUNTPE Rendezvous .....	58
4.1.14	Type 3 Tally Tag .....	58
4.1.15	LAQGSM Initialization.....	58
4.1.16	Special Tally Treatment FT PHL with Source Biasing.....	58
4.1.17	SP Normalization.....	58
4.1.18	BURN Card (n, $\gamma$ ) Cross Section.....	58
4.1.19	BURN Card MAT/MATVOL Reorder.....	59
4.1.20	Delayed/Decay Neutrons/Gammas Using CINDER.....	59
4.1.21	Residuals Tallies (FT8 RES).....	59
4.1.22	Pulse-Height Tallies (F8) .....	59
4.1.23	Pulse-Height Light Tallies (FT8 PHL) .....	60
4.1.24	Dependent Sources.....	60
4.1.25	MX Card for Protons .....	60
4.1.26	Photonuclear NRF .....	60
4.1.27	Muons.....	60
4.1.28	Photonuclear Model Physics for Kr, Th, U, and Pu.....	60
4.1.29	Duplicate Proton Elastic Scatter with Light-ion Recoil.....	61
4.1.30	Delayed Neutron and Gamma from Model Fission.....	61
4.2	Minor Problem Corrections.....	61
4.2.1	INTEL Compiler Workaround .....	61
4.2.2	LAQGSM Corrections.....	61
4.2.3	Compiler Workaround .....	62
4.2.4	Detector Tallies in Lattice Geometries.....	62
4.2.5	Burnup Duplicate ZAIDs .....	62
4.2.6	Source Particle Types Unrecognized in Dependent Distributions.....	62
4.2.7	Incorrect Warning Error for Detector Tallies .....	62
4.2.8	Choice of High-Energy Mode.....	62
4.2.9	Lost Particles Cause Crash .....	62
4.2.10	Tally Tagging Labels .....	63
4.2.11	Heavy Ion Direction Cosines .....	63
4.2.12	Cylindrical Mesh Tally .....	63

4.2.13	Stopping Power Bin Control .....	63
4.2.14	Revised GDR.dat .....	63
4.2.15	Muon Physics .....	63
4.2.16	Light Ion Production from Inelastic Collisions .....	63
4.2.17	Isomer Branching in Burnup.....	63
4.2.18	PTRAC Capture Events .....	64
4.2.19	Burnup Tier 3 Fission Products .....	64
4.2.20	KCODE Fission Source in MPI .....	64
4.2.21	CEM/LAQQSM.....	64
4.2.22	Delayed Neutron / Delayed Gamma Correction .....	64
4.2.23	Secondary Particle Arrays Increased .....	64
4.2.24	MPI Run Wall Clock Correction.....	64
4.2.25	Uninitialized or Out-of-Bounds Arrays .....	64
4.2.26	Intel 11.0 Compatibility .....	64
4.2.27	Table 38 Printing.....	65
4.2.28	Interactive Plotting Commands .....	65
4.2.29	Spontaneous Photon Zero-Volume Cells.....	65
4.2.30	TIR/TIC Bug Fix.....	65
4.2.31	Tally Multiplier (FM) Cards with Mesh Tallies.....	65
4.2.32	Burnup Corrections Regarding Fission Energy Boundaries .....	65
4.2.33	Torus Major/Minor Axes Ratio.....	65
4.2.34	CEM Upgrades.....	65
4.2.35	INCL Bug Fixes.....	65
4.2.36	IC=-99 Units Correction.....	65
4.2.37	Burnup Correction Sending Isomer Reaction Rates to CINDER90.....	65
4.2.38	Using a PHYS:N Card with Burnup.....	66
4.2.39	Burnup MODE N P .....	66
4.2.40	GBR Fix .....	66
4.2.41	Cinder Compatibility with FORTRAN Compilers.....	66
4.2.42	Recoil with Heavy Ions.....	66
4.2.43	SETRES Bug Fix .....	66
4.2.44	MSCAT Bug Fix .....	66
4.2.45	READ Card.....	66
4.2.46	MCTAL files if NPS>1e11 .....	67
4.2.47	NOACT=-2 for Electrons.....	67
4.2.48	Signal-to-Noise Ratio .....	67
4.2.49	Reading cindergl.dat.....	67
<b>5</b>	<b>FUTURE WORK .....</b>	<b>67</b>
	<b>APPENDIX A: IMPROVEMENT OF DNDG EMISSION-SPECTRA ACCURACY A-1</b>	
A.1	CDF Formulation .....	A-1
A.2	Analytic Integration.....	A-3
A.3	Discontinuation of Previous Normalization Procedure.....	A-3

## MCNPX 2.7.E 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.E, 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.E beyond MCNPX 2.6.0 are listed below. (Where applicable, the initials of the principal developers are shown in parentheses.<sup>1</sup>) Note that the arithmetic MCPLLOT capability and delayed-neutron/delayed-gamma capabilities are developmental. They are not backed by the MCNPX cash awards quality assurance program and must be used cautiously. However, these capabilities are considered of such significance that they are included. Recall also that as of version 2.6.0 total  $\nu$  (not prompt  $\nu$ ) is the default for fission neutrons. The new MCNPX 2.7.E 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)

---

<sup>1</sup> 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, D-5/Tech Source, Inc.); 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), Trevor A. Wilcox (TAW, LANL, D-5)

- LAQGS 3.03 upgrade (SGM)
- 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)<sup>1</sup>.

For approved users, beta test program versions may be downloaded from the MCNPX website.<sup>2</sup> 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](mailto: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,”<sup>3</sup> which comes with MCNPX from RSICC and is available to MCNPX beta testers from the MCNPX website.<sup>4</sup>

### *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.”<sup>5</sup> Similarly, features beyond MCNPX 2.5.0 that appear in MCNPX 2.6.0, are described in “MCNPX 2.6.0 Extensions.”<sup>6</sup>

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

All of the extended MCNPX capabilities are summarized in the MCNPX features list.<sup>7</sup>

## 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

---

<sup>1</sup> <http://rsicc.ornl.gov/>

<sup>2</sup> <http://mcnp.lanl.gov/beta>

<sup>3</sup> 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/](http://mcnp.lanl.gov/docs/MCNPX_2.6.0_Manual.pdf/).

<sup>4</sup> <http://mcnp.lanl.gov/>

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

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

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

finding anything that does not meet or exceed the capabilities of MCNPX 2.3.0 and MCNP4C3. 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.<sup>1</sup> A list of all winners since June 2001 can be found on the MCNPX website.<sup>2</sup>

## 2 DESCRIPTION OF NEW MCNPX FEATURES

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
- LAQGSM 3.03 upgrade

### 2.1 TALLY TAGGING

Tally tagging 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 (F1, F2, F4, F6, F7) and detector (F5) 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

```
FTn    TAG    a
```

---

<sup>1</sup> 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. MCNP/X 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.

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

where  $n$  is the neutron, photon, or electron 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 should be invoked):

- $a=1$  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. If a particle has multiple production events, the tag will be for the last production event. For example, a neutron undergoing fission followed by  $(n,2n)$  would have the  $(n,2n)$  tag. Otherwise the tag is lost with elastic scatter.

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

FU*n*     $bin_1$   $bin_2$  ...  $bin_N$  [NT]

where each tagging  $bin_i$  has the form CCCCCZZAAA.RRRRR. A user cell number is designated by CCCCC (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 2.1.2. 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  $^{12}\text{C}$ ). 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 FTn TAG option has not been used.

#### Special designations for CCCCCZZAAA:

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

#### Photon tally special designations for ZZAAA.RRRRR:

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

#### Electron tally special designations for ZZAAA.RRRRR:

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

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

ZZAAA.99999	delayed particles from fission of ZZAAA
-------------	---

The RRRRR reaction tag also includes all the MT reactions listed in Appendix G for neutrons, but selecting RRRRR is complicated by the inconsistencies of ENDF and other table data evaluations. For fission, RRRRR=18 will not always catch all fission reactions. For example, in  $^{239}\text{Pu}$  RRRRR=18, but in  $^{240}\text{Pu}$  RRRRR=19, 20, 21 and all three must be listed to catch  $^{240}\text{Pu}$  fission. Likewise, RRRRR=16 only tags  $(n,2n)$  reactions; RRRRR=17 must be used to get  $(n,3n)$  reactions. And then there are the exceptions. For example, photons from fission in  $^{235}\text{U}$  have the tag RRRRR=3, which is inelastic, and is also the tag of photons created by  $(n,xn)$ .

### 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  $^{235}\text{U}$  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 2<sup>nd</sup> 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  $^{235}\text{U}$  will be placed in the 2<sup>nd</sup> 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  $^1\text{H}$  will be put into the 01001.00102 bin; all remaining gammas from  $^1\text{H}$  interactions will be put into the 01001.00000 bin. All capture gammas from  $^{56}\text{Fe}$  will go into the 26056.00102 bin; all  $[n,n']$  1<sup>st</sup> level gammas will go into the 26056.00051 bin; all  $[n,n']$  2<sup>nd</sup> level gammas will go into the 26056.00052 bin; all deexcitation gammas from the spallation of  $^{56}\text{Fe}$  into  $^{52}\text{Cr}$  will go into the 26056.24052 bin; etc. All remaining gammas produced from  $^{56}\text{Fe}$  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
        10000000000.00000
```

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  $^{12}\text{C}$  in cell 1 will be put into the 2<sup>nd</sup> bin; all remaining photons produced from interactions with  $^{12}\text{C}$  in cell 1 will go into the 3<sup>rd</sup> bin. All capture gammas from  $^{56}\text{Fe}$  will go into the 4<sup>th</sup> bin; all remaining photons/gammas produced from interactions with  $^{56}\text{Fe}$  will go into the 5<sup>th</sup> bin. All  $[n,n']$  1<sup>st</sup> level gammas will be put into the 6<sup>th</sup> 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<sup>1,2</sup>

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 version 03.01 of these codes, the Fermi breakup model was used to calculate the disintegration of light nuclei but was not used at the pre-equilibrium, evaporation, and fission stages for an excited nucleus or a fission fragment with  $A < 13$ .

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  ${}^5\text{He}$ ,  ${}^5\text{Li}$ ,  ${}^8\text{Be}$ , and  ${}^9\text{B}$  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,” in other words, 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  ${}^4\text{He}$  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 Figure 1 and Figure 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.

---

<sup>1</sup> 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).

<sup>2</sup> 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.

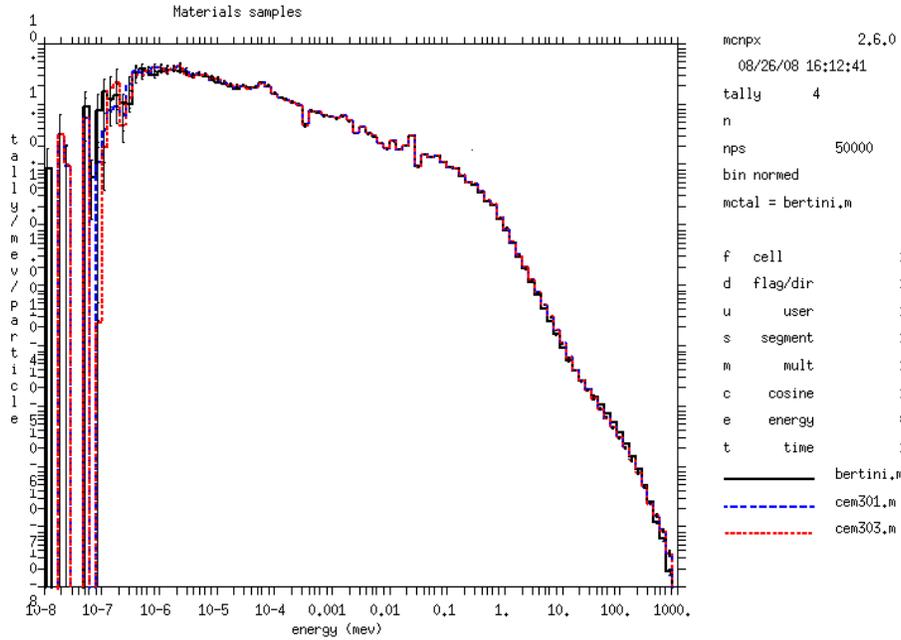


Figure 1. Neutron flux generated by an 800-MeV proton beam in LANSCE material samples. (Note that CEM 03.02 is mislabeled as “cem303” in the plot.)

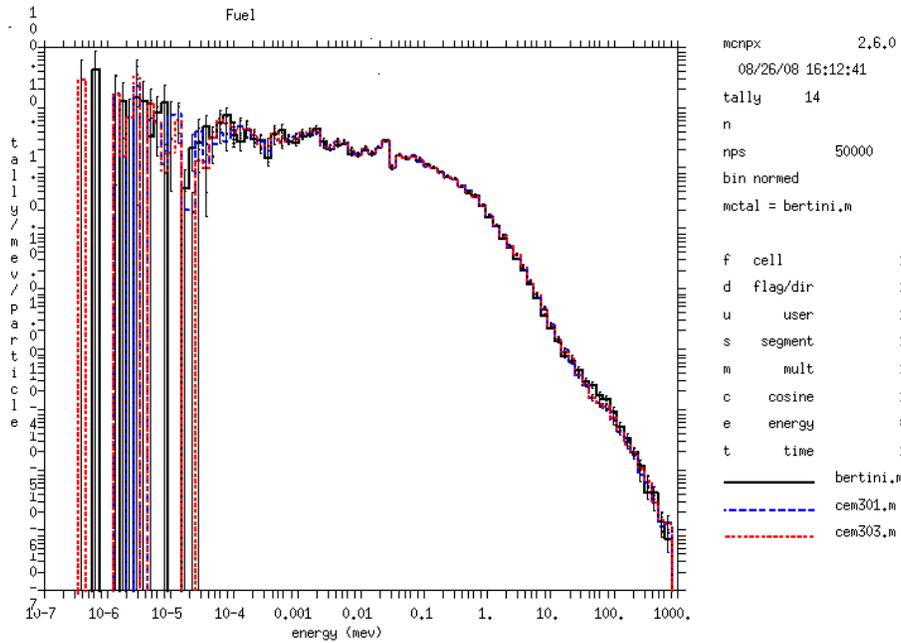


Figure 2. Neutron flux generated by an 800-MeV proton beam in LANSCE fuel sample. (Note that CEM 03.02 is mislabeled as “cem303” in the plot.)

## 2.3 MC PLOT GRAPHICS AND “HELP” COMMAND UPGRADES <sup>1</sup>

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  $\log_{10}$  axes for contour plots.

### 2.3.1 Graphics Upgrades

Among the graphical improvements are the following:

*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

---

<sup>1</sup> 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.

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.

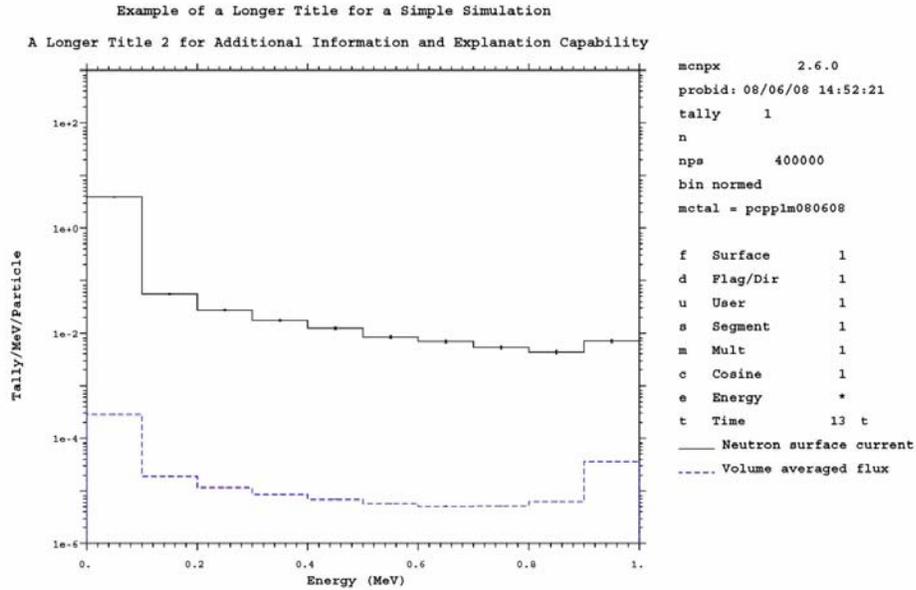


Figure 3. Upgraded MCPLLOT 2-D tally graphics.

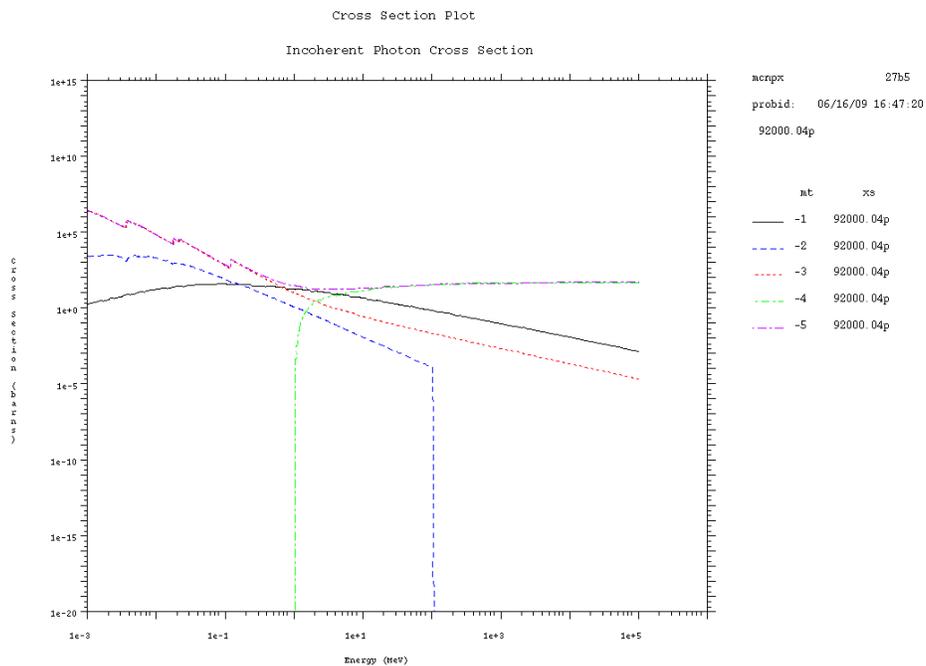


Figure 4. Upgraded MCPLLOT cross-section plot graphics.

*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.

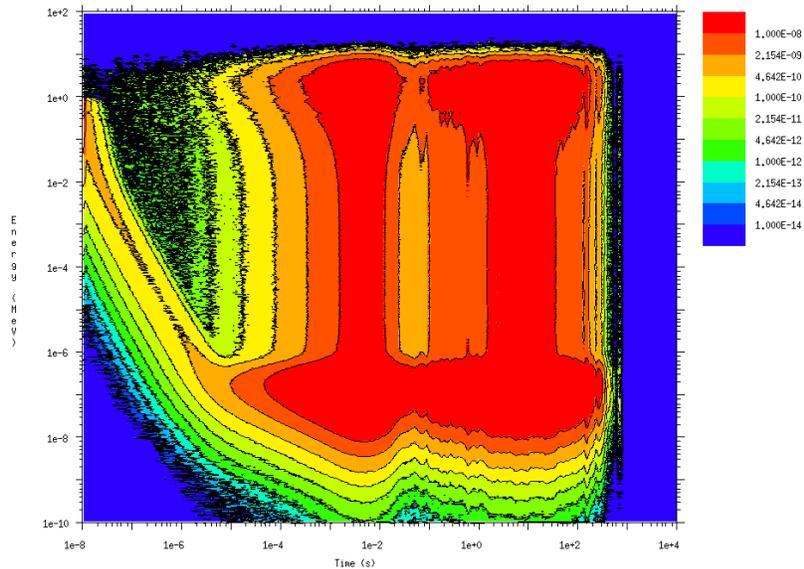


Figure 5. MCNPLOT log-scale contour plot.

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  $^{235}\text{U}$ . 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 MCNPLOT 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)" &
        ylims 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 MC PLOT “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 MC PLOT 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 MC PLOT 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 MCPLLOT 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 MCPLLOT plot from -5 to 25 shakes. The 1<sup>st</sup> 13 of a total 50 repetitions of distribution 11 (which are each two shakes in duration) are seen in the first part of the 2<sup>nd</sup> repetition of distribution 12.

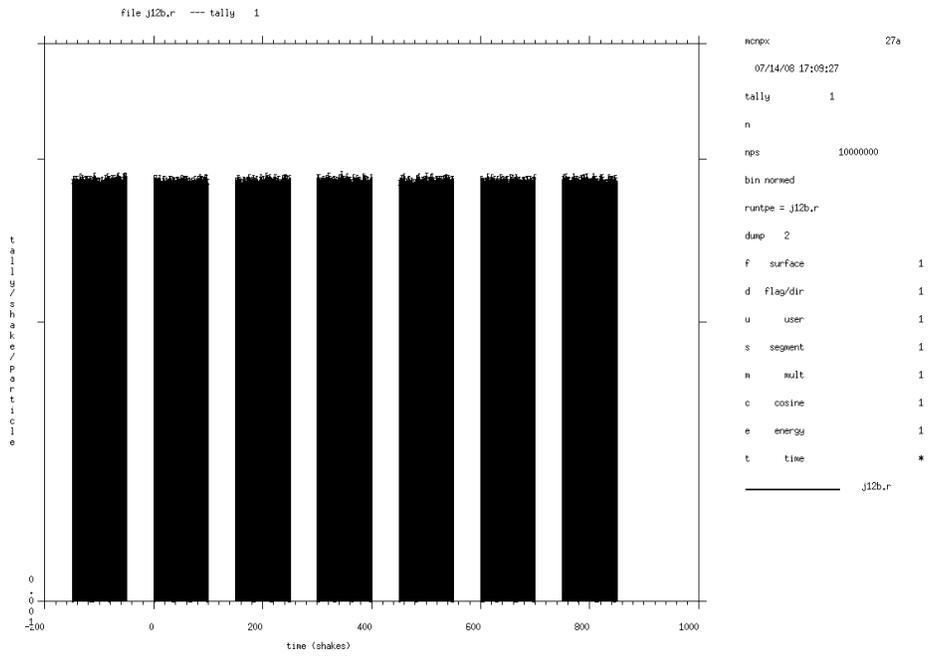


Figure 6. MCNPLOT plot of tally from -200 to 1000 shakes shows embedded pulses defined by distribution 12.

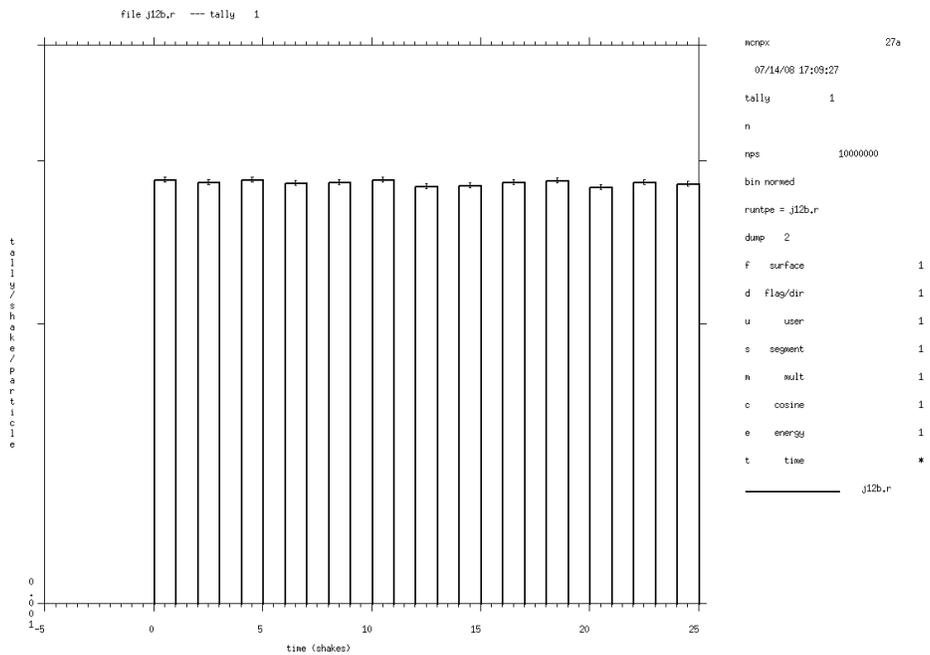


Figure 7. MCNPLOT plot of tally from -5 to 25 shakes, displaying embedded pulses defined by distribution 11.

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.

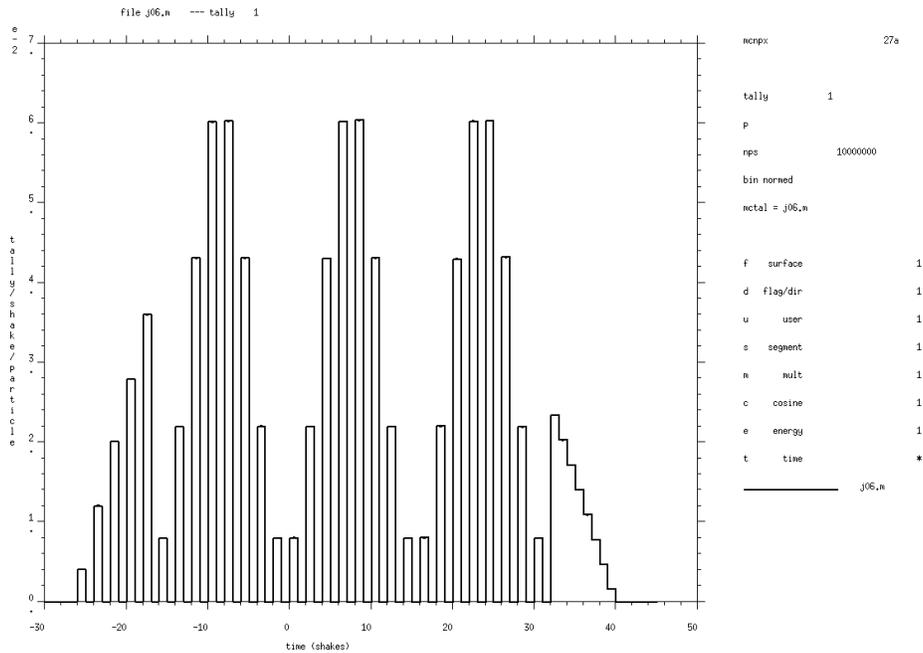


Figure 8. MCPLLOT plot of tally from -30 to 50 shakes.

## 2.5 STOPPING POWER ENERGY TABLE CONTROL

An 11<sup>th</sup> entry on the `PHYS:<pl>` card, where `<pl>` is any charged particle type, now controls the stopping power table energy spacing. This 11<sup>th</sup> 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:

$$E_{n-1} = E_n \times efac$$

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

<code>CBEG</code>	reference starting time in shakes (sh) (default=0)
<code>CFRQ</code>	frequency of cycling in 1/sh or 1/time width
<code>COFI</code>	dead time interval in shakes
<code>CONI</code>	alive time interval in shakes
<code>CSUB</code>	number of subdivisions to use within alive time (default=1)
<code>CEND</code>	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  $\mu\text{s}$  (`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 OPTION<sup>1</sup>

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,

$$\text{BEM} = \text{exn ey n bml}$$

where

- $\text{exn}$  is the normalized beam emittance parameter,  $\varepsilon_{nx}$ , for phase-plane coordinates  $x, x'$  ( $\pi$ -cm-radians),
- $\text{ey n}$  is the normalized beam emittance parameter,  $\varepsilon_{ny}$ , for phase-plane coordinates  $y, y'$  ( $\pi$ -cm-radians), and
- $\text{bml}$  is the distance from the aperture to the spot,  $L$  (cm); and

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

where

- $\text{ba1}$  is the beam aperture half-width in the  $x$  transverse direction,  $x_0$  (cm),
- $\text{ba2}$  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.

---

<sup>1</sup> 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)

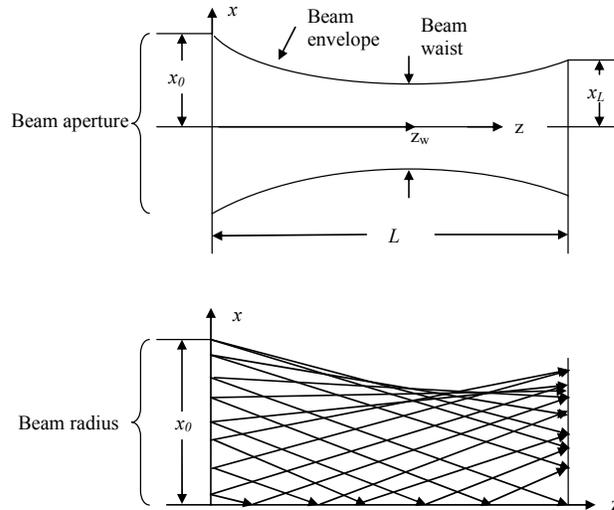


Figure 9. Beam envelope sketches. Upper: Beam projection in the drift region onto the  $x$ - $z$  plane in configuration space. The beam propagates from the aperture at  $z=0$  with an envelope parallel to the  $z$ -axis. The  $x$ - and  $y$ -directions are transverse to the  $z$ -axis. Lower: The beam 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 and explained in the associated caption.

### 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,  $\epsilon_{nx} = \epsilon_{ny} = 9.776 \times 10^{-1} \pi$ -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.

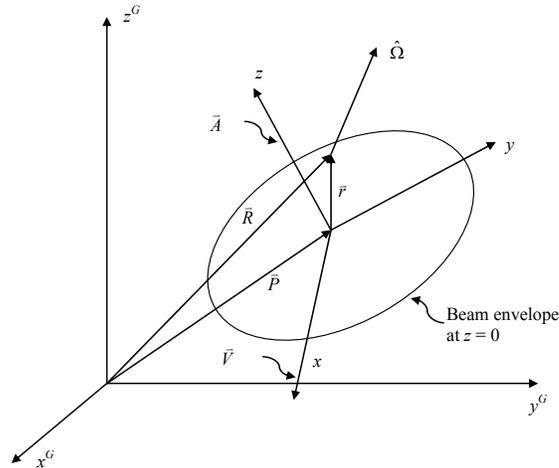


Figure 10. Locating and aiming a beam in MCNPX involves a transformation from local  $(x,y,z)$  to global  $(x^G, y^G, z^G)$  coordinates. The beam aperture is located in the local-coordinate  $x$ - $y$  plane at the entrance to the drift region ( $z=0$ ) at position  $\bar{P}$  (“POS”). The beam envelope 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.

```
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
```

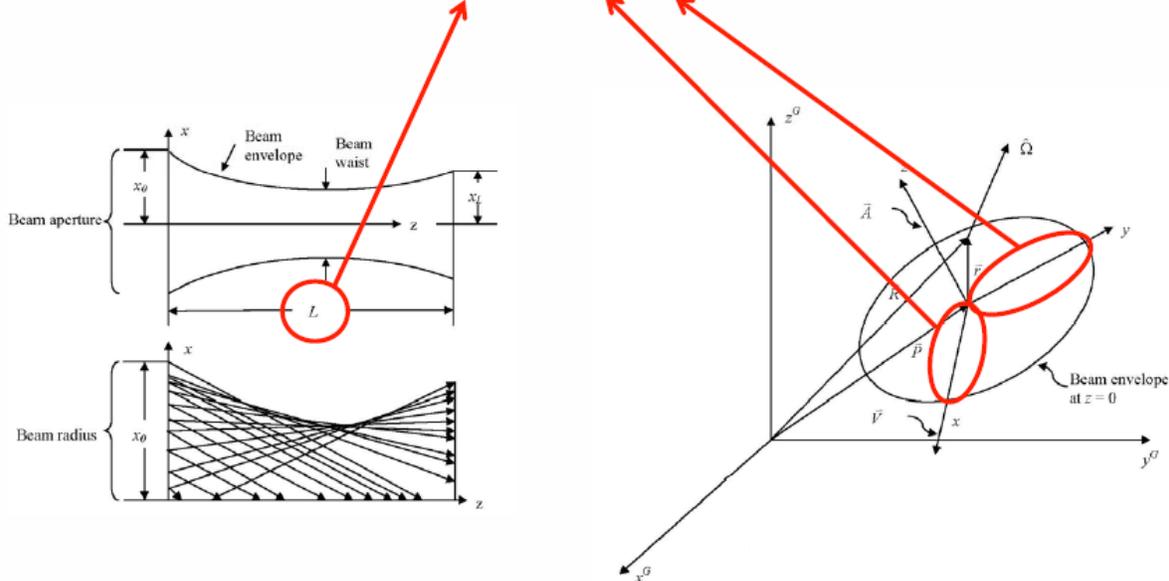


Figure 11. Description of a 100-MeV focused muon beam with a disk source positioned at POS=0 0 0 with a normal given by AXS=0 0 1 and an azimuthal orientation given by VEC=1 0 0. The desired drift-region length,  $L$ , is 100 m, and the beam aperture half-width in both the  $x$ - and  $y$ -directions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

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.

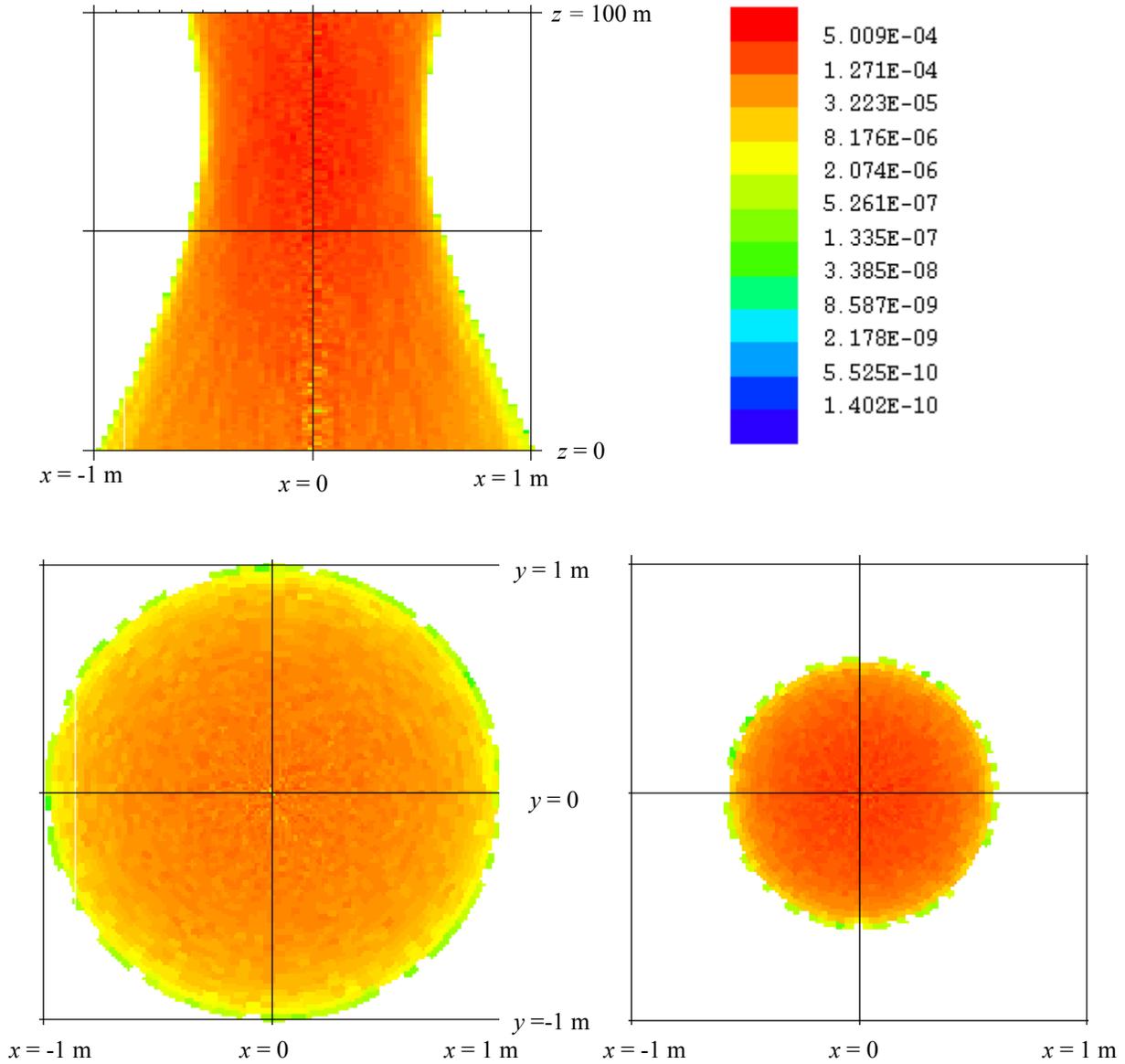


Figure 12. Mesh tally of the muon flux in a void. Upper: Mid-beam side view at  $y=0$ . Note that the window extent is exaggerated in the  $z$ -direction to better illustrate the beam axial profile. Lower left: Beam radial profile at the aperture ( $z=0$ ). Lower right: Beam radial profile at the desired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

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

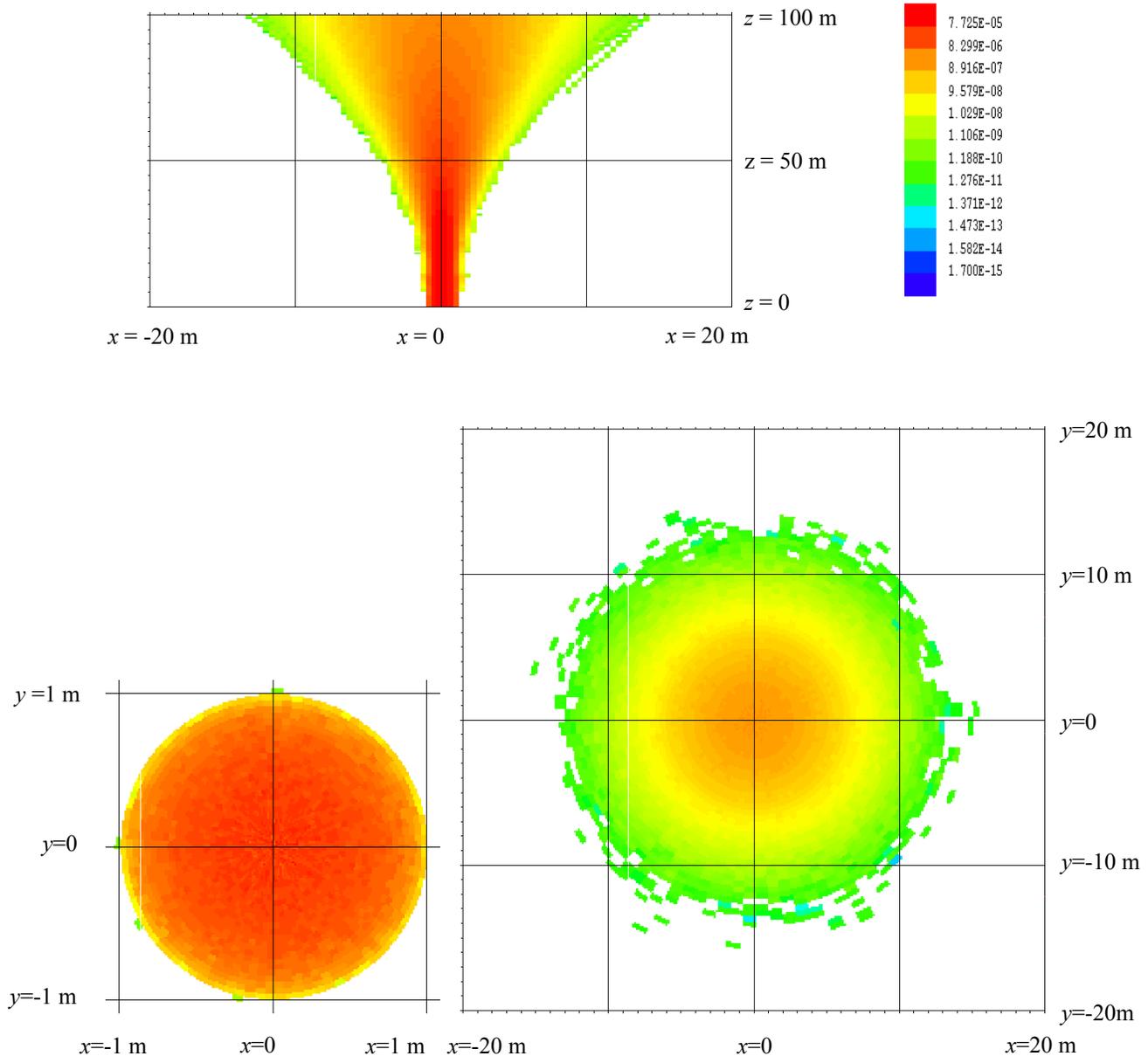


Figure 13. Mesh tally of the muon flux in air. Upper: Mid-beam side view at  $y=0$ . Note that the window extent is exaggerated in the  $z$ -direction to better illustrate the beam axial profile. Lower left: Beam radial profile at the aperture ( $z=0$ ). Lower right: Beam radial profile at the desired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

### 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.

## 2.9 LLNL MULTIPLICITY

The LLNL fission model<sup>1</sup> is an optional fission treatment that enables prompt gammas from photofission, correlation of neutrons and photons from fission, and neutron and photon multiplicity so that the number of emitted particles is not just the integer closest to the average value.

### 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. The 7<sup>th</sup> 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 (as opposed to when *fism*=0). This enables coincidence counting of photofission secondaries. A message in the OUTF file confirms the use of LLNL multiplicity.

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

The LLNL photofission has three advantages over the default ACE treatment:

- 1) prompt photofission gammas are produced;
- 2) photonuclear neutrons and gammas are correlated; and
- 3) the correct multiplicity of photofission neutrons and gammas is used. The number of secondaries is correctly sampled rather than being the number just above or below the average.

---

<sup>1</sup> Jerome M. Verbeke, Chris Hagmann, Doug Wright, "Simulation of Neutron and Gamma Ray Emission from Fission and Photofission," Lawrence Livermore National Laboratory report UCRL-AR-228518 (May 11, 2010) <http://nuclear.llnl.gov/simulation/>

The exact modeling of the photofission process enables coincidence counting of photofission neutrons and gammas.

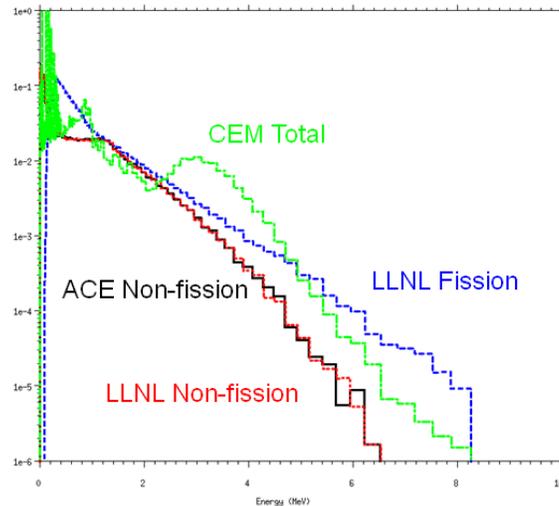


Figure 14. Resultant gamma-ray emissions from 12-MeV x-rays directed onto  $^{235}\text{U}$ . Y-axis is the gammas/interaction/MeV/source particle. Note the deficiency of the ENDF VII photonuclear libraries that do not emit gammas from fission.

### 2.9.2 LLNL Neutron Fission Multiplicities

If the 6<sup>th</sup> 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. This option cannot be used with delayed-neutron biasing (see the 4<sup>th</sup> entry, `dnb`, on the `PHYS:N` card and the `DN` keyword on the `ACT` card). A message to the `OUTP` file confirms the use of LLNL multiplicity.

#### Neutron-induced fission

The main advantage of the LLNL neutron fission model is that neutron-induced photons are correlated with the fission event.

The LLNL fission model is the only MCNPX method emitting spontaneous fission prompt photons. These are neglected in the MCNPX default `FMULT` spontaneous fission source.

The LLNL fission model multiplicities (number of neutrons and photons per fission) are an alternative to the other MCNPX fission multiplicity treatments with `fism=0, 1, 2, 3, or 4` on the `PHYS:N` card. Although the total number of fission neutrons produced is about the same for the ACE data and LLNL model, the production of 0, 1, 2, 3, ... neutrons from fission—that is, the individual multiplicities—are about 5% different. The factorial moments are also about 5% different between ACE and LLNL—approximately a ten standard deviation difference appears in sample runs for  $^{235}\text{U}$  and  $^{239}\text{Pu}$ . ACE had twice as many fissions with no fission neutrons compared to LLNL for  $^{239}\text{Pu}$  and 50% more for  $^{235}\text{U}$ .

The LLNL fission multiplicity model (`PHYS:N 3J -1 J 5` as above and `MODE N P`) produces neutron-induced photons correlated with fission events. Gamma production from

neutron-induced fission is significantly different between ACE and LLNL as shown in Figure 15 and Figure 16. From the summary table:

	----- 239-Pu -----		----- 235-U -----	
	ACE	LLNL	ACE	LLNL
Photon tracks from neutrons	2000000	5465251	1000000	2239147
Photon weight from neutrons	6.6648	6.1619	2.0732	3.3124
Photon energy from neutrons	6.6315	6.3619	1.7437	2.8552

The LLNL model ran about 30% slower than ACE.

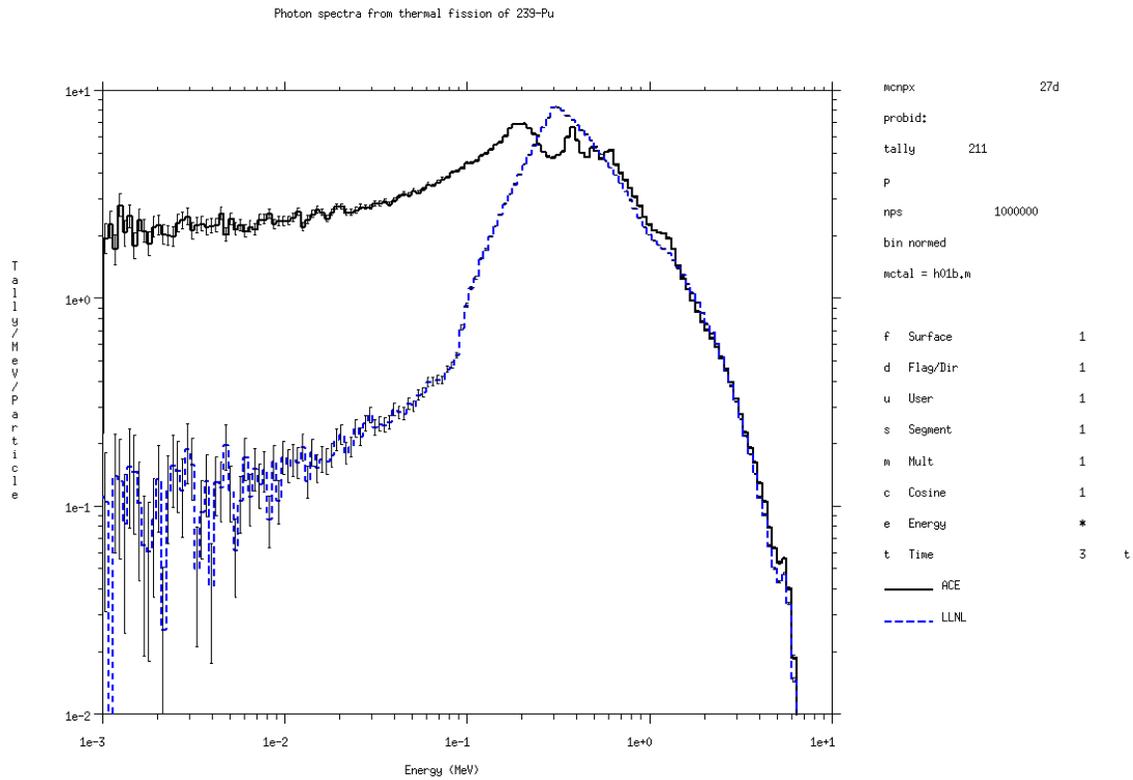


Figure 15. Photon energy spectra of induced gammas from <sup>239</sup>Pu thermal induced fission.

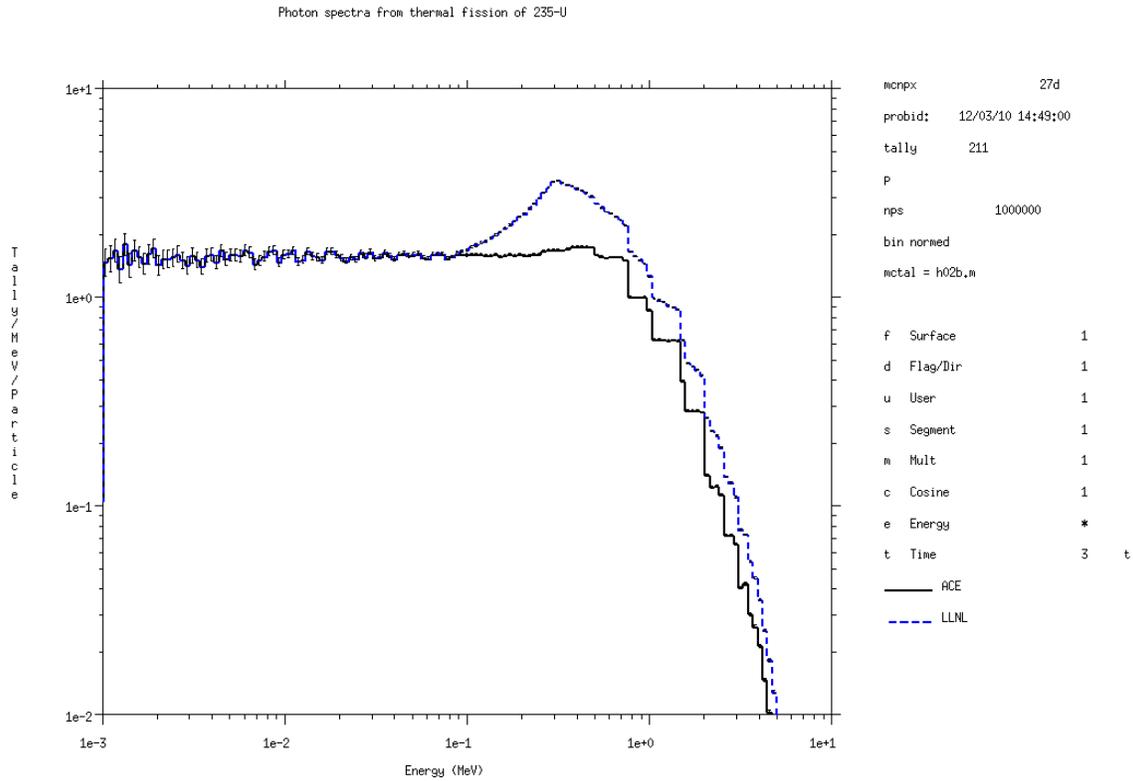


Figure 16. Photon energy spectra of induced gammas from  $^{235}\text{U}$  2-MeV induced fission.

Spontaneous fission

The LLNL fission model is the only MCNPX method emitting spontaneous fission prompt photons. These are neglected in the MCNPX default FMULT spontaneous fission source.

The spontaneous fission neutron spectra are statistically the same between LLNL and FMULT. Consequently the heating is the same. The average number of spontaneous fission neutrons,  $nu$ , is statistically the same for all but  $^{252}\text{Cf}$  where it is  $3.77248\text{E}+00\ 0.0003$  for LLNL fission and  $3.75657\text{E}+00\ 0.0003$  for ACE table physics, a 0.42% difference with 0.03% relative error. The multiplicity distributions and moments are nearly identical for  $^{233}\text{U}$ ,  $^{238}\text{U}$ ,  $^{238}\text{Pu}$ ,  $^{240}\text{Pu}$ ,  $^{242}\text{Pu}$ ,  $^{242}\text{Cm}$ , and  $^{244}\text{Cm}$ . They are statistically different, but similar (within 1%) for  $^{252}\text{Cf}$ . But they are quite different for  $^{232}\text{Th}$ ,  $^{232}\text{U}$ ,  $^{234}\text{U}$ ,  $^{235}\text{U}$ ,  $^{236}\text{U}$ ,  $^{237}\text{Np}$ ,  $^{239}\text{Pu}$ ,  $^{241}\text{Pu}$ ,  $^{241}\text{Am}$ , and  $^{249}\text{Bk}$ . The biggest differences are for  $^{239}\text{Pu}$ .

## 2.10 ARITHMETIC MC PLOT OPTIONS<sup>1</sup>

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 MC PLOT 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 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 <i>fn</i>	Read saved arithmetic tallies from file <i>fn</i> ; if <i>fn</i> does not exist, print an error message to the screen
RZMCTAL <i>fn</i>	Write all saved arithmetic tallies that have been created in the MC PLOT session so far to file <i>fn</i> ; if <i>fn</i> 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

---

<sup>1</sup> 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.

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 MCPLLOT “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 MCPLLOT 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 is no restriction 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 MCPLLOT 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, by default the operation 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 latter 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 MCXPLOT 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 MCPLLOT 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 MCPLLOT, 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 MCPLLOT 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 17. Unless overridden by user-specified title lines in MCPLLOT, the default title will be the operation line that creates the plot.

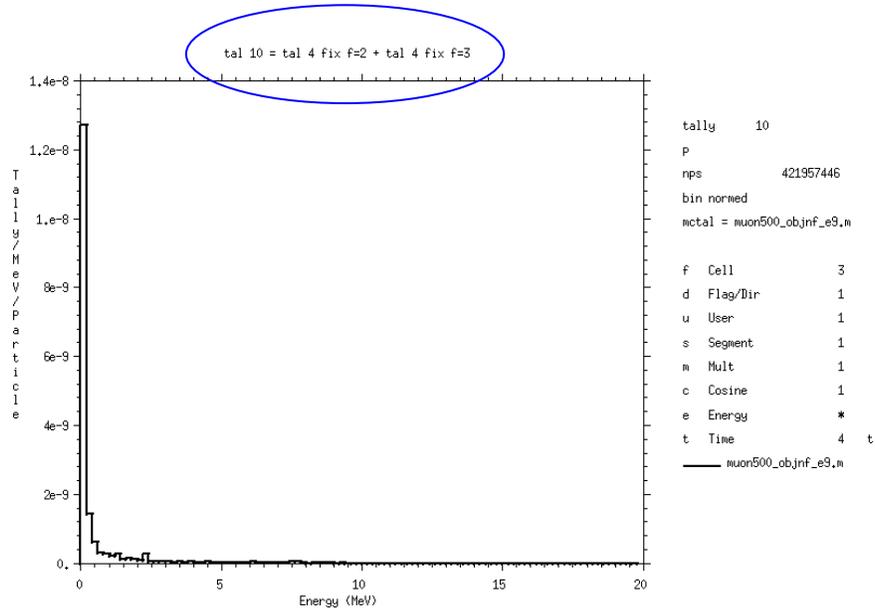


Figure 17. The title of this plot, circled in blue, is given by the default value: the operation that created the plot. This title can be replaced by using the `TITLE n` command available in MCPLLOT.

#### 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 18. The commands used to create the plot below are provided for completeness.

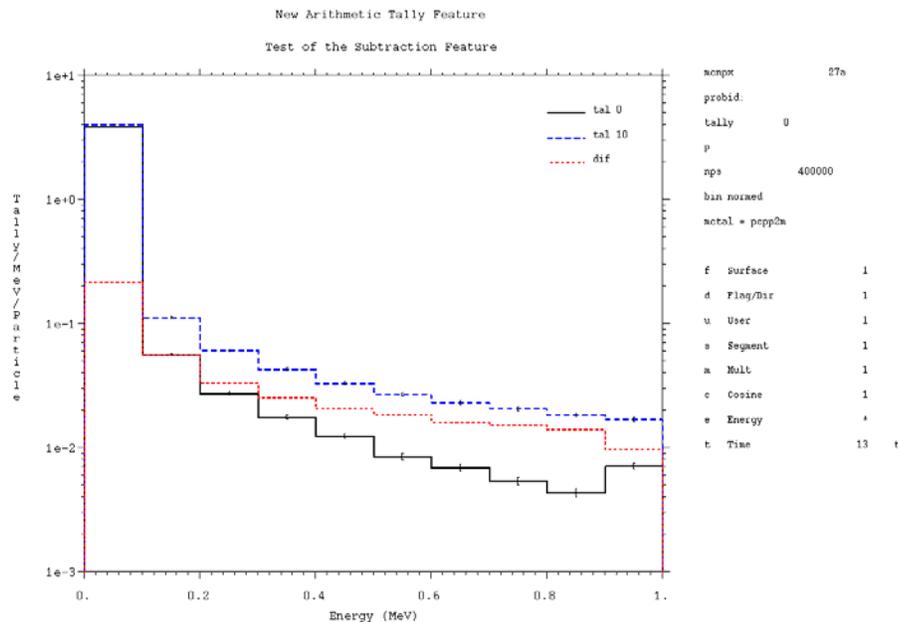


Figure 18. Three arithmetic tallies are coplotted, tal 0, tal 10, and tal 30, where tal 30 is the red dotted line representing the calculated difference between tal 0 and tal 10.

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 particle 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 5<sup>th</sup> 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 *nhb*; 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.,  $1 \times 10^8$  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 2<sup>nd</sup>, 3<sup>rd</sup>, and 4<sup>th</sup> regions, respectively. The tally numbers and f-bin values for these regions work the same as for the first region.

The energy bins for the four regions are as follows:

```

Energy (E):    1st region
User (FU):     2nd region
Segment (FS):  3rd region
Cosine (C):    4th region

```

For example:

```

f8:h,t,s      ( 2 3 4 5 )
ft8          PHL 3 6 1 16 1 26 1
              3 6 2 16 2 26 2
              3 6 3 16 3 26 3
              3 6 4 16 4 26 4
e8           0 20 NT
fu8          0 20 NT
c8           0 20 NT
fs8          0 20 NT
fq8          s c e u

```

### 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).

## 2.14 LAQGSM 3.03 UPGRADE

The LAQGSM model physics package was upgraded from version 03.01 to the most recent version, version 03.03<sup>1</sup> (dated 12/02/2010). This version is the same as exists in MCNP6. As compared to version 03.01, more of the internal data has been fitted to experimental results and bugs have been corrected. Among the many other improvements include:

- A recently improved version<sup>2</sup> of the time-dependent intranuclear cascade model developed initially in Dubna, and often referred simply in the literature as the Dubna intranuclear Cascade Model, DCM,<sup>3</sup> using the Quark-Gluon String Model (QGSM)<sup>4 5 6 7</sup> to describe elementary interactions at energies above 4.5 GeV;
- Fission calculated using an improved version of GEM2 that is an extension by Shiori Furihata of the RAL fission model of Francis Atchison;
- Changes in the calculation of the fission cross sections; several routines by Furihata from GEM2 were slightly modified in CEM03.03/LAQGSM03.03; some bugs found in GEM2 were fixed; and
- The Fermi breakup model code used in LAQGSM03.03 and in CEM03.03 was developed in the group of Prof. Barashenkov at JINR, Dubna.<sup>8</sup> Some notable changes in the Fermi breakup model are:
  - The decay of some unstable light fragments like <sup>5</sup>He, <sup>5</sup>Li, <sup>8</sup>Be, <sup>9</sup>B, etc., that were produced by the original Fermi breakup model;
  - Several bugs/uncertainties observed in the original version were fixed; this solved the problem of the production of "nucleon stars" like "nuclides" *xn* and *yp* allowed by the original version; and

---

<sup>1</sup> S. G. Mashnik, et al., "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, Feb. 4–8, 2008, ICTP, Trieste, Italy; LANL Report LA-UR-08-2931; FNAL Report FERMILAB-CONF-08-322-APC; E-print arXiv:0805.0751 [nucl-th].

<sup>2</sup> S. G. Mashnik, K. K. Gudima, Mol. Baznat, A. J. Sierk, R. A. Prael, N. V. Mokhov, LANL Report, LA-UR-06-1764, Los-Alamos (2006).

<sup>3</sup> V. D. Toneev, K. K. Gudima, Nucl. Phys. **A400** (1983) 173c.

<sup>4</sup> N. S. Amelin, K. K. Gudima, V. D. Toneev, Sov. J. Nucl. Phys. **51** (1990) 327.

<sup>5</sup> N. S. Amelin, K. K. Gudima, V. D. Toneev, Sov. J. Nucl. Phys. **51** (1990) 1730.

<sup>6</sup> N. S. Amelin, K. K. Gudima, V. D. Toneev, Sov. J. Nucl. Phys. **52** (1990) 172.

<sup>7</sup> N. S. Amelin, CERN/IT/ASD Report C~RN/IT/99/6, Geneva, Switzerland (1999).

<sup>8</sup> N. Amelin, "Physics and Algorithms of the Hadronic Monte-Carlo Event Generators. Notes for a Developer," CERN/IT/ASD Report CERN/IT/99/S, Geneva, Switzerland (1999); "GEANT4, Users' Documents, Physics Reference Manual," last update: 08/04/1999; <http://wwwinfo.cern.ch/asd/geant4/G4UsersDocuments/UsersGuides/PhysicsReferenceManual/html/PhysicsReferenceManual.html/>.

- The incorporation of the Fermi breakup model at the pre-equilibrium and evaporation stages of reactions (earlier, it was used only after the INC).

LAQGS 03.03 thus describes nuclear reactions of interest to spallation applications better than earlier versions.

### 3 MCNPX 2.7.E 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.<sup>1</sup>

- 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 <sup>235</sup>U 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)

---

<sup>1</sup> 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, D-5/Tech Source, Inc.); 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), Trevor A. Wilcox (TAW, LANL, D-5)

- NCIA upgrade (JSH)
- M0 library specification card (MLF/LSW)
- new cinder.dat (GWM)
- minor enhancements

### 3.1 SPONTANEOUS PHOTON FEATURES

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.

#### 3.1.1 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 “SP” 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 SP source is specified, the code will create an optional table 44 that summarizes the activities of the materials in the problem.

#### 3.1.2 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
```

#### 3.1.3 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 the PAR=SP or PAR=ZZZAAA ERG=0 options, either 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  $1 \times 10^{18}$  seconds ( $\sim 3.17 \times 10^{10}$  years) are treated as stable.

### 3.1.4 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 (SPn) 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
```

### 3.1.5 SPn w Source Probability Option—Automatic Source Weight Adjustment

A new source probability option has been added. The “SPn 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, as is done for all MCNPX source distributions; 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 “SPn 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 source distribution normalization will be done as described above and the weight adjustment 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 SP<sub>n</sub> 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
s11 L sf
sp1 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

### 3.2.1 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.

### 3.2.2 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.

### 3.2.3 Unlimited MATMOD Changes

Additional dynamic dimensioning now permits an unlimited number of user-specified concentration changes (MATMOD 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 linear energy transfer special tally treatment, 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 ICRP-60 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 (see the DF card IU option). This effective-dose function uses a lookup of the stopping power,  $S(E,p)$ , to create a multiplier of the absorbed dose. To request this dose function, specify IC=99 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 of quality factors,  $Q$ , 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=2 fac=-3
```

This example uses the ICRP-60 dose function to produce a tally that gives results in Sv/h (assuming the source weight is particles/s) for alpha particles in cell 77.

**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 MCNPX 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 7<sup>th</sup> 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.

MCNPX 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
sil  L (4<2[-1:1 -2:2 -3:3]<1)
spl      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). The user may choose to not create delayed particles from fission and/or non-fission events (NONE); to create delayed neutrons (N), delayed photons (G), delayed betas (E), and/or delayed alphas (A); or to create all delayed particles (ALL).

Additional keywords provide a convenient user interface to control the DNDG feature. The keywords include DN, to choose use of libraries, models, or a combination for delayed neutrons (previously controlled using the 4<sup>th</sup> entry on the PHYS:N card); DG, to select line vs. multigroup data for delayed gammas (previously controlled using the 6<sup>th</sup> entry on the PHYS:P card); THRESH, to specify the fraction of gammas that are retained, consequently saving computer time because insignificant gammas are not followed; DNBIAS, to establish delayed neutron bias (previously controlled using the 4<sup>th</sup> 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`, 4<sup>th</sup> entry, and the `PHYS:P`, 6<sup>th</sup> 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 <sup>235</sup>U DELAYED NEUTRON SPECTRUM

Previously, through MCNPX 2.7.B, MCNPX used a <sup>235</sup>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 FOR ROC SPECIAL TALLY

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 multiple bins to be specified for each entry:

- 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. For many isotopes, the necessary nuclear data is not available to allow a precise calculation of the muonic x-ray spectra using MUON/RURP. Therefore, 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:

- xmurnum*=-1 use only x-ray literature data (isotopes without literature values do not emit muonic x-rays)
- xmurnum*=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, <sup>56</sup>Fe elastic recoils from 20-MeV neutrons are tallied and displayed in Figure 19.

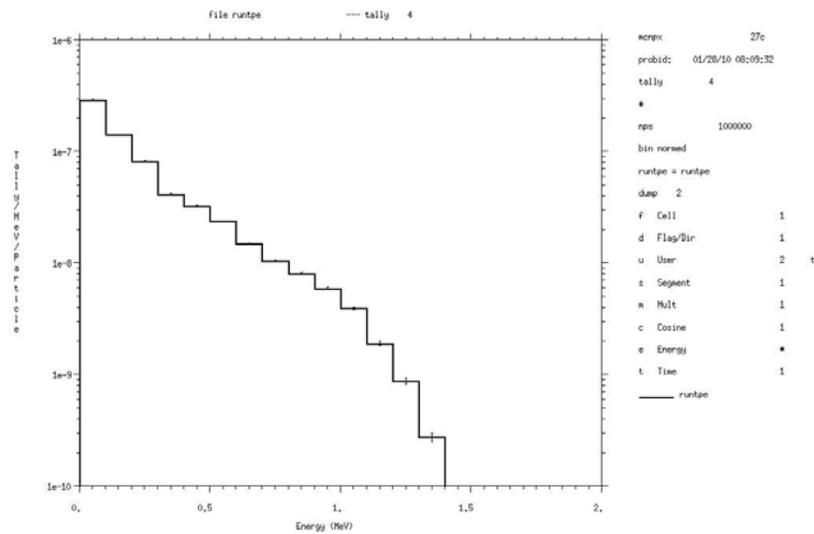


Figure 19. Flux tally of  $^{56}\text{Fe}$  elastic recoils from 20-MeV neutrons.

### 3.18 EXACT ENERGY INTEGRATION IMPROVES DELAYED GAMMA SPECTRA<sup>1,2</sup>

Recall that equating the DG keyword on the ACT card to LINES (or, equivalently, the 6<sup>th</sup> 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 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.

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

<sup>1</sup> 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)

<sup>2</sup> 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)

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  $^{235}\text{U}$  and  $^{239}\text{Pu}$ <sup>†</sup> 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 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  $^{239}\text{Pu}$  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.

---

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

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 20.

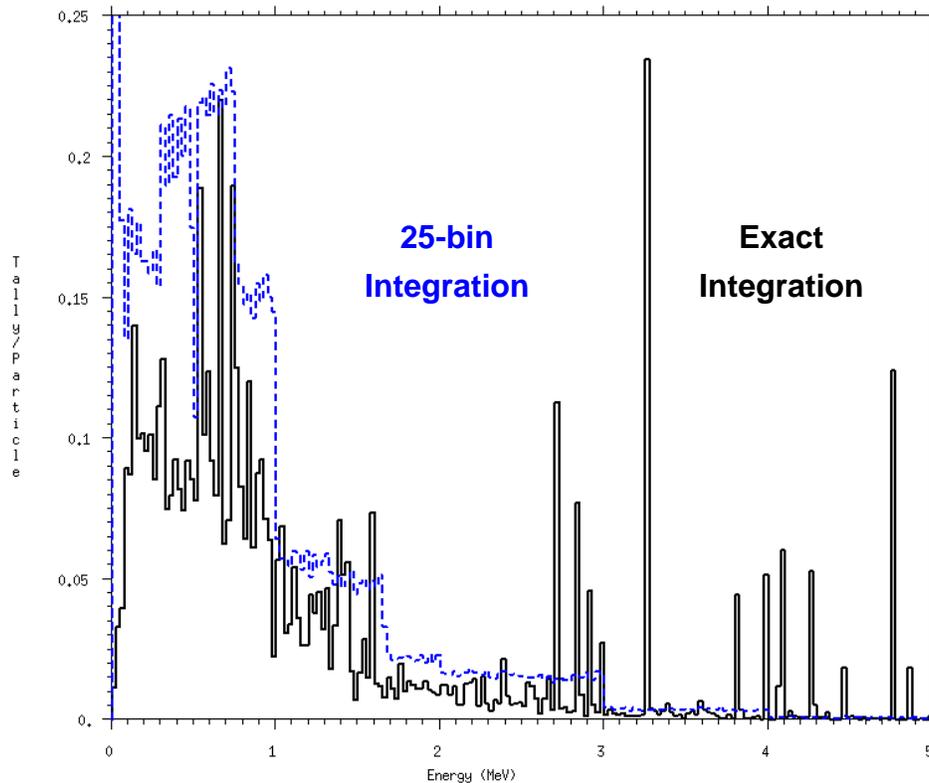


Figure 20. Delayed gamma spectrum emitted from  $^{235}\text{U}$  struck by thermal neutrons. The delayed spectrum using a multigroup sampling method (`ACT DG=MG`) is compared to that using exact delayed-gamma sampling (`ACT DG=LINES`).

### 3.19 DELAYED NEUTRON/DELAYED GAMMA CALCULATIONS USING IMPLICIT CAPTURE

Previous to MCNPX 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 MCNPX 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 3<sup>rd</sup> entry on the `CUT:<p1>` 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  $6 \text{ \AA}^{-1}$ . 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://mcnpx.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 22<sup>nd</sup> 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,<sup>1</sup> 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

---

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

products that are generated when  $^{235}\text{U}$  and  $^{239}\text{Pu}$  are subjected to thermal-neutron fission. No user control for fission exists in MCNPX.

### 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.<sup>1</sup> 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 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 MCNPX 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 MCNPX 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.

## 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 5<sup>th</sup> column of output now provides the `ZAID` identifier of the spontaneous fission nuclide. A value of 0 appears if the source is not spontaneous fission, i.e., `PAR=SF`. The 6<sup>th</sup> column contains the `ZAID` of the first induced fission; the 7<sup>th</sup>, that of the second induced fission; the 8<sup>th</sup>, that of the third induced fission; and the 9<sup>th</sup>, that of the last fission before capture, either induced or spontaneous. If `DBCN(23)>0`, only the four-column output, like that in MCNPX 2.7.B, is provided.

## 3.24 FULL ZAID IDENTIFIERS ON MX CARD

Full `ZAID` 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`).

---

<sup>1</sup> J. W. Durkee, M. R. James, G. W. McKinney, H. R. Trellue, 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 (2009)

**Example:**

```

m1      8016 1.0
        82206 10.0
        nlib=.60c
        hlib=.24h
        pplib=.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 MCNPX 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 MCNPX 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, <sup>3</sup>He, and alphas) per incident neutron to be created at each neutron elastic scatter event with light nuclei H, D, T, <sup>3</sup>He, and <sup>4</sup>He. 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  $0 < rec1 < 1$  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, and limiting the minimum increment in  $m$  to 0.001,

if	$rec1 = 0$	Light ion recoil is off, NCIA is off (default)
if	$.001 < rec1 < 1.001$	Light ion recoil makes $rec1$ ions from elastic scatter
if	$1.001 < rec1 < 2.001$	Light ion recoil makes $rec1-1$ ions from elastic scatter; NCIA ions from neutron capture*
if	$rec1 = 3$	Light ion recoil is off, NCIA ions from neutron capture*
if	$3.001 < rec1 < 4.001$	Light ion recoil makes $rec1-3$ ions from elastic scatter, NCIA ions from neutron capture <sup>†</sup>
if	$rec1 = 5$	Light on recoil is off; NCIA ions from neutron capture <sup>†</sup>

\* Table data ion production will be used if possible

<sup>†</sup> 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 NEW CINDER.DAT

The new cinder.dat file has been updated with a new set of photofission (PF) fission-product (FP) yields. The delayed neutron (DN) production is more in line with expectation for 12-MeV gammas incident on  $^{235}\text{U}$  (0.014 neutrons/fission instead of the previous 0.020 neutrons/fission). The neutron induced-fission neutron/fission values are in the 0.017 range. The integral delayed gamma (DG) production remains essentially unchanged (although the spectrum is somewhat different). The differences between the old and new cinder.dat delayed-neutron and delayed-gamma spectra are shown in Figure 21 and Figure 22.

The new cinder.dat photofission yields are taken from the GEF code.<sup>1</sup> The cinder.dat neutron-induced fission yields continue to be based on ENDF/B-VI. The MCNPX 2.7.D cinder.dat had a fairly serious problem with the CEM-based FP yields. About half of the 60 yield sets integrated

---

<sup>1</sup> Schmidt, K. H., Jurado, B., "General Model Description of Fission Observables," CENBG CNRS/IN2P3 Report, France, October (2010). Available at <http://www.cenbg.in2p3.fr/GEF>

to values above 2.0 and the MCNPX sampling algorithm requires it to integrate to 2. Thus, there was an under-sampling of the high-Z (2nd) hump of the FP peak.

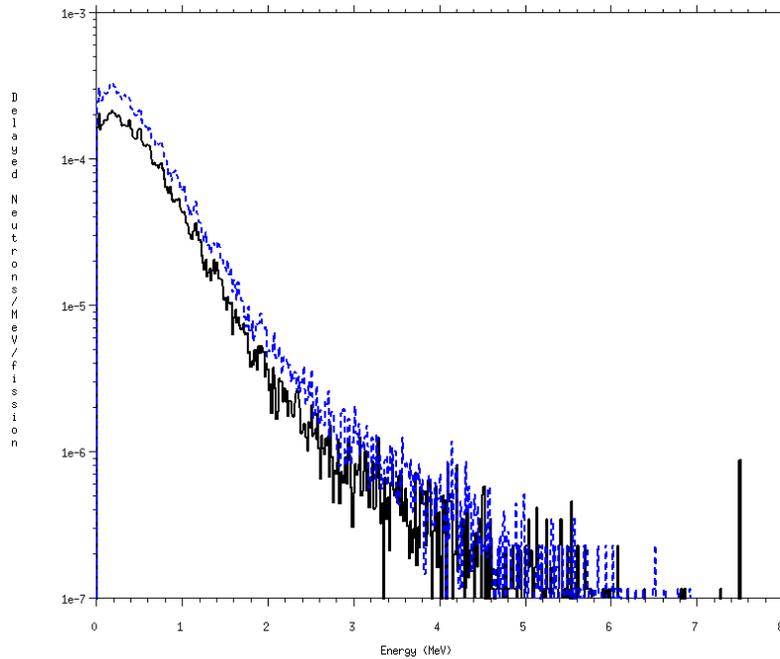


Figure 21. 12-MeV photons into  $^{235}\text{U}$ , first collision only. Blue is old cinder.dat photofission yield set (MCNPX/CEM) and black is new cinder.dat yield set (GEF). The integral for delayed neutrons is 0.020 n/f for the old cinder.dat and 0.014 n/f for the new cinder.dat.

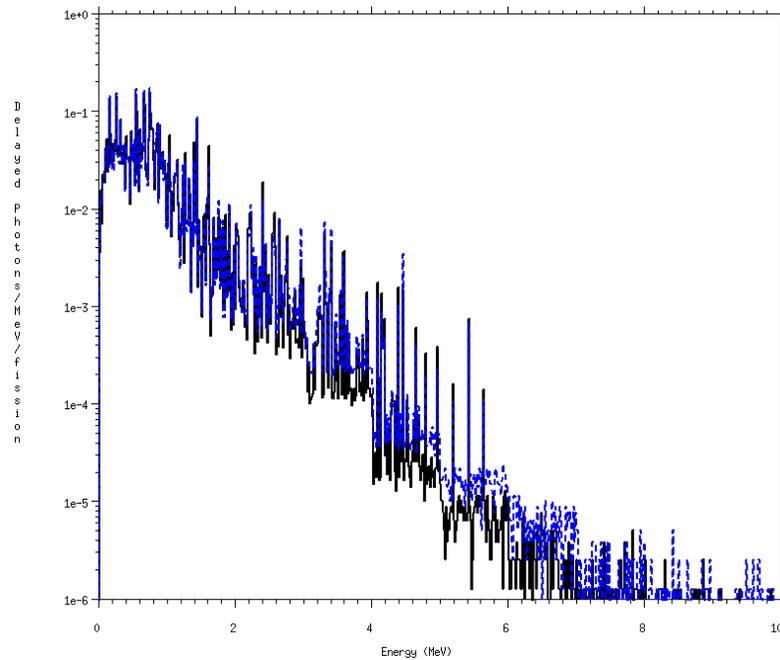


Figure 22. 12-MeV photons into  $^{235}\text{U}$ , first collision only. Blue is the old cinder.dat photofission yield set (MCNPX/CEM) and black is new cinder.dat yield set (GEF). The integral for delayed photons is 5.61  $\gamma$ /f for the old cinder.dat and 5.58  $\gamma$ /f for the new cinder.dat.

### 3.29 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)
- The tracking switches have been changed (so that a new version of MCNPX can track an old one). The following tracking switches were available in MCNPX 2.6.0:
  - `dbcn(20)`, which caused tracking with MCNPX 2.5.0;
  - `dbcn(21)`, which caused tracking with MCNPX 2.5.E; and
  - `dbcn(25)`, which turned off the Eric Pitcher/Bob Little  $S(\alpha,\beta)$  broadening enhancement in MCNPX 2.6.0.

The only tracking switch now available is `dbcn(26)`, which causes MCNPX 2.7.E to track MCNPX 2.7.D. To fully track previous versions it is necessary to have the LAQGSM (laqmod31.F), cinder.dat, GDR.dat, LLNL Fission (LLNFission.cc and fissionEvent.h) appropriate to the version where tracking is desired. (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 5<sup>th</sup> 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 MCNPX 2.7.C, MCNPX offers improved support for Solaris operating systems.
- AIX/xlf is supported beginning in MCNPX 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.
- Increased the limit of CPUs for MPI parallel runs from 515 to 1027. (MRJ)
- The photofission fission product yields are selected from three data sets depending upon the incident photon energy. In MCNPX 2.7.E these are changed from  $0 < E < 10$ ,  $10 < E < 50$ , and  $50 < E$  to the following:  $0 < E < 7.5$ ,  $10 < E < 12$ , and  $12 < E$ . (GWM)

## 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 2.7.A corrections to MCNPX 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 *comb* 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 2.7.B corrections to MCNPX 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 ZAID 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 (*SP<sub>n</sub> 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 *SP<sub>n</sub> 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 spon\_phot routine. (MRJ)

#### *MCNPX 2.7.C corrections to MCNPX 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 ( $A+300+100*\text{state}$ ) 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 2.7.D corrections to MCNPX 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  $SBn$  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, $\gamma$ ) Cross Section

The (n, $\gamma$ ) reactions rates being reported to CINDER90 were actually total absorption rates. To accelerate the computation of (n, $\gamma$ ) reaction rates, total absorption was used as an approximation for (n, $\gamma$ ). For many nuclides, total absorption is roughly equal to (n, $\gamma$ ); however, in some light ions, such as  $^{10}\text{B}$ , (n, $\alpha$ ) dominates capture, and therefore total absorption is not roughly equal to

( $n,\gamma$ ). MCNPX now calculates the actual ( $n,\gamma$ ) 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)

#### *MCNPX 2.7.E corrections to MCNPX 2.7.D*

#### **4.1.20 Delayed/Decay Neutrons/Gammas Using CINDER**

Delayed neutrons from ACE-library table physics are robust. A number of bugs have been corrected for the delayed neutron/gammas models (ACT card or some PHYS:N and PHYS:P options) to create these particles from activation and decay using CINDER.

A fudge factor of 0.88 for correcting integral gamma emission (DNG\_MODEL) was removed. [MCNPX 2.7.D only] Integral gamma emission was too low. (MRJ)

An out-of-bounds error was corrected that could cause wrong answers when certain arrays overflowed. (DNG\_MODEL) (MRJ/JWD)

Bad emission spectra occurred from time cutoffs. Some photon emission spectra peaks were incorrect because the problem time cutoff was used instead of the maximum time in the CINDER library when constructing the total gamma emission cumulative density function (CDF). (JWD)

Delayed neutron/gamma models used an incorrect angular distribution scattering law (IPSC) with point detectors (F5) and DXTRAN (DXT).

#### **4.1.21 Residuals Tallies (FT8 RES)**

Fission product residuals: The residual list for binary fission was incorrectly initialized (MODULE CINDER). Affected FT RES. (JWD)

Residual tallies failed in the presence of other tallies. [MCNPX 2.7.D only] (MRJ)

#### **4.1.22 Pulse-Height Tallies (F8)**

F8 tallies with photonuclear bias: This is now a fatal error, but can be run with the fatal option. Previously it caused silent wrong answers. Answers are still wrong when run with the fatal option. (GWM)

F8 tallies and unresolved resonances: The warning message for unresolved resonances in conjunction with F8 tallies was improperly called. Analog capture is now turned on as appropriate. Note that the unresolved resonance treatment applies to neutrons only and that FT8 tallies for neutrons are illegal in MCNP5. In MCNPX neutron unresolved resonances are appropriate with FT8 CAP tallies, usually FT8 RES tallies, and often FT8 PHL tallies. (GWM)

#### 4.1.23 Pulse-Height Light Tallies (FT8 PHL)

FT8 PHL tallies with four regions: An out-of-bounds error occurred with the 4-fold FT8 PHL tallies in the unusual case when the 4<sup>th</sup> region, which used segment bins, had a tally go beyond the bin range. JBIN overflows the array (NTBB) for counting values that exceed maximum bin values [MCNPX 2.7.D only] (MRJ)

Print Table 30 FT8 PHL tally bin printout with more than two PHL regions: The energy, user, segment, and cosines bins with an F8 PHL tally are now printed correctly. In MCNPX 2.7.D the printout was wrong for the new segment and cosine bin capabilities. As before, the energy and user bins are printed out. But if the PHL is more than 2-fold then the segment and cosine bins are printed as PHLs and PHLC bins in Print Table 30 and the code does not try to give a segment facet number or require the cosine bins to be between -1 and 1. (JSH)

#### 4.1.24 Dependent Sources

The DS Q source capability was incorrect in some cases with DXTRAN/detectors (MRJ)

#### 4.1.25 MX Card for Protons

The MX card incorrectly treated protons (STUFF). Affected  $MXn:H$  only. (MRJ/MLF)

#### 4.1.26 Photonuclear NRF

Interpolation of ACE library photonuclear data was incorrect in rare cases with nuclear resonance fluorescence (NRF) when partial photonuclear cross sections did not add up due to narrow NRF peaks. These reactions are now resampled. Affected photonuclear production with the new .30u photonuclear libraries only. (GWM)

#### 4.1.27 Muons

The emission of k-shell electrons was corrected. (RCJ/MRJ)

The time delay of the electrons from muon decay, that is, the time signature of the decays, was off by a factor of ten. The times were updated in units of shakes, when the unit of time for the LAHET Code System (LCS) routines is nanoseconds. The secondary particles from the muon annihilation also had emission times shortened by the erroneous muon decay time. This affects all muon electron time-dependency. (MRJ)

Low-energy muon reactions failed to interact and the message “unable to interact in CEM: itype=12, energy=0.000,a=...z=...” frequently occurred. Sometimes there was such a volume of these messages that they would interfere with network traffic. These messages arise when a nuclear excitation (in the form of a virtual photon) is sent to CEM with an energy that is very small, less than  $\sim 500$  eV. These virtual photons come from the muon annihilation excitation function which uses a linear interpolation and the lowest energy bin starts at zero. A random number which is very small will produce very small excitation values. The correction is that if the energy  $<1$  keV, the muon disintegration is resampled. (MRJ)

#### 4.1.28 Photonuclear Model Physics for Kr, Th, U, and Pu

The GDR.dat data file (in data.tar.gz accompanying MCNPX) contained obsolete data which affected model physics photonuclear production in these isotopes. (FXG/JSH)

Values were incorrect for the Kr ( $Z=36$ ) isotopic data in GDR.dat in data.tar.gz for MCNPX 2.6.0, MCNPX 2.7.C, MCNPX 2.7.D, and in all versions of the source directory v27x/Data/CEM.

Values were incorrect for Th, U, and Pu ( $Z=90, 92,$  and  $94$ ) isotopic data in GDR.dat in data.tar.gz for MCNPX 2.7.A and MCNPX 2.7.B. These data were “temporarily” changed to force the photofission branching provided by the BOFOD library for CEM2K. Now that MCNPX 2.7.D uses CEM03, the photoabsorption is still in use but the photofission corrections are obsolete (not present and very likely not needed).

#### **4.1.29 Duplicate Proton Elastic Scatter with Light-ion Recoil**

When a proton data library includes secondary particle production by elastic scatter and light-ion recoil is turned on for protons (PHYS:H card), the proton elastic scatter was duplicated both in the library table physics and the light-ion recoil model. In particular, for protons interacting with  $^3\text{He}$  (as in the case of 2003.70h),  $h+2003 \rightarrow h+s$ , ( $h = \text{proton}$ ,  $s=3\text{-He}$  secondary particle) the  $^3\text{He}$  particle duplicated any  $^3\text{He}$  created by proton elastic recoil. The correction is as follows: if proton elastic recoil is on and an isotope’s secondary particle production produces its light ion from elastic scatter, only the light-ion recoil secondary ion is transported. (JSH)

#### **4.1.30 Delayed Neutron and Gamma from Model Fission**

Delayed neutron and delayed gamma production was included only for one of the two fission product residuals produced in model physics fissions (neutron, photon, and proton-induced fissions). The error was in MCNPX versions 2.6.C through 2.7.D and does not affect table physics fission. Consequently, delayed neutron and gamma production from model fission were significantly underestimated by as much as a factor of two. This underestimation is observable in the neutron summary table under “delayed fission” and in the photon summary table under “particle decay.” It is also evidenced in fewer late-time neutron and photon tallies. (GWM)

## **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 2.6.0 corrections to MCNPX 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 Gunging, (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 2.7.A corrections to MCNPX 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 2.7.B corrections to MCNPX 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 11<sup>th</sup> entry on the PHYS:<pl> card, where <pl> is any charged particle type, was documented for MCNPX 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)

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

#### 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 MCNPX 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 2.7.B. (JSH/MRJ)

*MCNPX 2.7.C corrections to MCNPX 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 2.7.D corrections to MCNPX 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)

*MCNPX 2.7.E corrections to MCNPX 2.7.D***4.2.45 READ Card**

If when writing an encrypted file using the READ card ENCODE option, the file already existed, the encoded file was renamed (“familied”) and a warning was sent to the terminal.

Consequently the user could write an encrypted file of a different name than intended with no way to check. (This problem had a very bad effect on the MCNPX test sets.) To correct this problem, if the filename already exists when trying to write (encode) a new readfile, the following error message is issued:

“bad trouble error”: “cannot encode existing read file: filename” (JSH)

READ card filenames or passwords containing capital letters could not be read [MCNPX 2.7.D only] and is now corrected. (MLF)

Markers in the OUTF output file that indicate the beginning and end of READ files were incorrect and have corrected [MCNPX 2.7.D only] (JSH).

#### **4.2.46 MCTAL files if NPS>1e11**

MCTAL files written by runs with more than 1e11 histories had “\*\*\*\*\*” in the *nps* (number of particles started, or histories) field of the tally fluctuations chart and thus could not be read. The correction is to use scientific notation instead of integer notation if *nps*>1e11. (MRJ)

#### **4.2.47 NOACT=-2 for Electrons**

The NOACT=-2 option (8<sup>th</sup> entry on the LCA card) has been enabled for electrons. Thus electron sources and progeny are treated consistently with other particle types. The NOACT=-2 option causes all source particles to immediately collide and all progeny to be transported through a void and escape. This option is used to compute and tally double differential cross sections with an F1 tally or to compute and tally residual nuclei with an F8 tally in conjunction with the FT RES option. (GWM)

#### **4.2.48 Signal-to-Noise Ratio**

The signal-to-noise ratio is a component of the figure-of-merit (FOM) of a tally that is used to normalize the differences in FOM arising from using computers of different speeds. Using this ratio enables comparison of different variance reduction efficiencies across different computer platforms. For problems with very short running times, the signal-to-noise ratio could sometimes be printed as zero. Now the correct value in the limit of short running times is printed so that the signal-to-noise ratio is always computed. (JSH)

#### **4.2.49 Reading cindergl.dat**

The ENDF/B-VII.0 cindergl.dat file contains more nuclides than the ENDF/B-VII.0 CIDNER.dat file. As cindergl.dat was read in, a corresponding nuclide from cinder.dat was sought. If none existed, the index nn90 was set to 3401. This created an array indexing problem. To correct this problem, nuclides that are in cindergl.dat but not in cinder.dat are skipped as they are read in. (TAW)

## **5 FUTURE WORK**

MCNPX has been merged with MCNP5 to create MCNP6. All future development will be with MCNP6.

## APPENDIX A

### APPENDIX A: IMPROVEMENT OF DNDG EMISSION-SPECTRA ACCURACY

In versions of the MCNPX code prior to MCNPX 2.7.D, DNDG calculations used the trapezoidal rule numerical algorithm to perform the CDF time-integration.<sup>†</sup> In MCNPX 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  $\tilde{i}^{\text{th}}$  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  $\tilde{n}^{\text{th}}$  radioactive decay species associated with the  $\tilde{i}^{\text{th}}$  fission product (atoms/m<sup>3</sup>),  $\lambda_{\tilde{i};\tilde{n}}$  is decay constant for  $\text{FP}_{\tilde{i}}$  and nuclide  $\tilde{n}$  (s<sup>-1</sup>), 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

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

where the Kronecker delta function is

$$\delta_{\tilde{k}} = \begin{cases} 0 & \text{for } E \neq E_{\tilde{k}} \\ 1 & \text{for } E = E_{\tilde{k}} \end{cases}, \quad (4)$$

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

---

<sup>†</sup> 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

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

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

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

where

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

and

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

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 MCNPX 2.7.D, 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,  $N_{\tilde{i}:j,\tilde{j}}(t) = N_{\tilde{i}:0,\tilde{j}} e^{-\lambda_{\tilde{i}} t}$ ,  $\tilde{j} = 1$ . 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  $^{60}\text{Co}$  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  $\gamma$ /decay. MCNPX 2.7.D calculates 1.9988  $\gamma$ /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 MCNPX 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, MCNPX 2.7.D discontinues the renormalization of DG line-emission data using the ebf6 factor.