

**MCNPX EXTENSIONS
VERSION 2.5.0**

by

John S. Hendricks
Gregg W. McKinney
Laurie S. Waters
Teresa L. Roberts
Harry W. Egdorf
Joshua P. Finch
Holly R. Trelue
Eric J. Pitcher
Douglas R. Mayo
Martyn T. Swinhoe
Stephen J. Tobin
Joe W. Durkee
Los Alamos National Laboratory

Franz X. Gallmeier
Oak Ridge National Laboratory

Jean-Christophe David
CEA-Saclay, Gif-sur-Yvette, France

William B. Hamilton
HQC Professional Services

Julian Lebenhaft
Paul Scherrer Institute, Switzerland

April 2005

CONTENTS

	Page
1.0. INTRODUCTION.....	1
1.1. MCNPX Extensions.....	1
1.2. Guarantee.....	3
1.3. Availability.....	3
2.0. PHYSICS EXTENSIONS.....	4
2.1. Neutrons: PHYS:N.....	4
2.1.1. Mix and Match (TABL).....	5
2.1.2. Fission Multiplicity (FISM).....	6
2.1.3. Light-Ion Recoil (RECL).....	7
2.2. Photons: PHYS:P.....	8
2.2.1. Photonuclear Model Physics (ISPN).....	8
2.2.2. Photon Doppler Broadening (NODOP).....	9
2.3. Protons: PHYS:H.....	10
2.4. Charged Particles: PHYS:x.....	11
2.5. Mix-and-Match Nuclide Replacement: MX.....	11
2.6. Physics Models: LCA.....	14
2.6.1. Inline Generation of Double Differential Cross Sections and Residual Nuclei.....	14
2.6.2. CEM2k Physics Model (ICEM).....	16
2.6.3. INCL4/ABLA (Cugnon/Schmidt) Physics Models (ICEM).....	17
2.7. INCL4 Options: LCC.....	18
2.8. ABLA Fission-Evaporation Model: LEA.....	18
2.9. Improved S(α,β) Treatment: MT.....	18
2.10. User Specification of Multiplicity Constants: FMULT.....	19
2.10.1. Nuclides without Transport Cross Sections.....	20
2.10.2. Nuclides without Multiplicity Data.....	21
3.0. SOURCE FEATURES.....	21
3.1. Particle-Type Specification: SDEF.....	22
3.2. Positron Sources: SDEF.....	22
3.3. Spontaneous Fission Sources: SDEF.....	22
3.3.1. Spontaneous Fission Physics.....	22
3.3.2. Normalization of Summary and Tally Information.....	23
3.3.3. Fission Multiplicity Output.....	23
3.4. Multiple Particles on SDEF Card.....	25
3.4.1. Source Particle Type as the Independent Variable.....	25
3.4.2. Source Particle Type as a Dependent Variable.....	25
3.4.3. Additional Capabilities and Cautions.....	25
3.4.4. Tally and Summary Table Normalizations.....	26
3.5. Sources on Cylindrical Surfaces: SDEF.....	26
3.5.1. Examples.....	27
3.5.2. Additional Information and Cautions.....	27

3.6. Repeated Structures Source Specifications: SI	28
3.7. Translated Sources with Dependence	28
4.0. TALLY FEATURES	28
4.1. Pulse-Height Tallies with Variance Reduction.....	29
4.1.1. Future Work	29
4.2. Default Dose Functions (DF).....	29
4.3. Lattice Tally Speedup (F)	31
4.4. Radiography Tally (FIP, FIR, FIC).....	32
4.4.1. Pinhole Radiography	32
4.4.2. Transmitted Image Projection	32
4.5. Photonuclear and Proton Reaction Multipliers (FM).....	32
4.6. Expanded Cosine Specification (C).....	33
4.7. Pulse-Height Light Tally with Anticoincidence: FT8 PHL.....	33
4.8. Coincidence Capture Tally (FT8 CAP)	35
4.8.1. Restrictions.....	36
4.8.2. Interpreting Capture Tally Output.....	36
4.8.3. FT8 Capture Tallies with Time Gating	39
4.8.4. Possible Future Extensions of FT8 CAP Option.....	42
4.9. Residual Nuclei Tally: FT8 RES	43
5.0. OTHER INPUT FILE EXTENSIONS	44
5.1. Logarithmic Interpolation	44
5.2. Auxiliary Input File and Encryption.....	45
5.2.1. Reading from an Auxiliary File.....	45
5.2.2. Suppressing Input Printing.....	45
5.2.3. Encryption of Input	46
5.3. HISTP File Size Control	46
5.4. DXTRAN Improvements.....	47
5.4.1. Detectors with Model Physics (Isotropic Approximation).....	47
5.4.2. Detector/DXTRAN Underflow Control (DBCN)	47
5.5. PTRAC for All Particles and for Coincidence Counting.....	47
5.5.1. PTRAC for All Particles (PTRAC).....	47
5.5.2. PTRAC Capture File for Coincidence Counting (PTRAC)	48
6.0. GRAPHICS	49
6.1. Color Contour Plots for Mesh Tallies, Radiography Tallies, and Lattice Tallies.....	49
6.1.1. User Interface for Contour Tally Plots	50
6.1.2. Mesh Tally Contour Plot Example	52
6.1.3. Radiography Tally Coutour Plot Example	58
6.1.4. Lattice Tally Plot Examples	60
6.1.5. Other Notes and Future Work	61
6.2. Enhanced Color Geometry Plots: 64-Color Plotting and Shading by Cell Parameters.....	61
6.3. i,j,k Lattice Index Labeling.....	62
6.4. Weight-Window-Generator Superimposed Mesh Plots.....	63
6.4.1. Geometry Plot of Weight-Window-Generator Superimposed Mesh	63
6.4.2. Example.....	64

6.5. Proton and Photonuclear Cross-Section Plots.....	65
6.5.1. Photonuclear Cross-Section Plots	65
6.5.2. Proton Cross-Section Plots.....	67
6.6. Pause Command.....	67
7.0. PARALLEL PROCESSING.....	67
7.1. Distributed Memory Multitasking for the Entire Energy Range of All Particles	67
7.2. MPI Multiprocessing	67
7.3. MPI Speedup for Criticality Calculations.....	68
7.3.1. DXTRAN and Detector Tracking Differences.....	68
7.3.2. User Interface Changes for Both Sequential and Parallel KCODE Problems ..	69
7.3.3. User Interface Changes for Parallel KCODE Problems.....	69
7.3.4. Compiler and Operating System Problems for Parallel KCODE Problems	69
8.0. COMPILING, CONFIGURATION, AND INSTALLATION	70
8.1. F90 Modularity and Dynamic Memory Allocation	70
8.2. F90 Autoconfiguration.....	70
8.3. 64-Bit-Integer Support.....	70
8.3.1. Recompilation Requirements for 64-Bit Integers	71
8.3.2. Additional Notes.....	71
8.4. NAG/IBM/INTEL F90 and Compiler Extensions.....	71
9.0. SUMMARY OF MCNPX CAPABILITIES SINCE MCNP4B (BY VERSION).....	72
10.0. FUTURE WORK.....	74
11.0. BIBLIOGRAPHY	75
11.1. Code Manuals	75
11.2. Code Version Release Announcements	75
11.3. Reports	76
11.4. Papers	76
12. ACKNOWLEDGMENTS	79

MCNPX EXTENSIONS, VERSION 2.5.0

ABSTRACT

MCNPX is a Fortran 90 Monte Carlo radiation transport computer code capable of tracking 34 particle types at nearly all energies. It is a superset of MCNP4C and MCNPX2.3.0. This document describes the capabilities beyond these constituent codes.

1.0. INTRODUCTION

MCNPX is a Fortran 90 (f90) Monte Carlo radiation transport computer code that transports 34 particle types, including four light ions, at nearly all energies. MCNPX stands for MCNP eXtended. It is a superset of MCNP4C3 and MCNPX2.3.0 and has many capabilities beyond these constituent codes. These capability extensions enhance physics, sources, tallies, graphics, and infrastructure.

MCNPX is a production computer code for modeling the interaction of radiation with matter, and its quality is guaranteed. See Section 1.2 regarding the MCNPX guarantee and cash awards. MCNPX is used widely around the world. See Section 1.3 for availability.

MCNPX is backward compatible with MCNP4C3 and older MCNPX (2.3.0 and earlier) versions. Old input files still work and usually track, giving identical results. The new MCNPX capabilities involve some changes, but mostly extensions, to the input cards.

1.1. MCNPX Extensions

Each successive version of MCNPX adds new capabilities and modernizes the code for new hardware, operating systems, and compilers. The extensions of MCNPX beyond MCNP4C and MCNPX2.3.0 now are listed with the initials of the principal developers shown in parentheses.* (Section 9 contains a complete list of new capabilities since MCNP4B grouped according to version release.)

Physics

- Seamless transport of 34-particle types at nearly all energies by mixing and matching of nuclear data table and model physics (JSH),
- CEM2k physics (SGM/AJS/FXG),

* Kenneth J. Adams (KJA), Nate A. Carstens (NAC), Leland L. Carter (LLC), Skip Egdorf (HWE), Thomas M. Evans (TME), Jeffrey A. Favorite (JAF), Franz X. Gallmeier (FXG), John S. Hendricks (JSH), H. Grady Hughes (HGH), Julian Lebenhaft (JL), Robert C. Little (RCL), Stepan G. Mashnik (SGM), Douglas R. Mayo (DRM), Gregg W. McKinney (GWM), Eric J. Pitcher (EJP), Richard E. Prael (REP), Teresa L. Roberts (TLR), Arnold J. Sierk (AJS), Edward C. Snow (ECS), Avneet Sood (AS), Martyn T. Swinhoe (MTS), Stephen J. Tobin (SJT), Laurie S. Waters (LSW), Christopher J. Werner (CJW), and Morgan C. White (MCW).

- INCL4/ABLA physics models (JCD/JSH),
- Extension of neutron model physics below 20 MeV (JSH),
- Fission multiplicity (JSH),
- Light-ion recoil (JSH),
- Inline generation of double differential cross sections and residuals (JSH),
- Photon Doppler broadening (from MCNP5) (AS/GWM),
- Weight-window generator (WWG) and exponential transform for model physics (FXG/ JSH), and
- Improved $S(\alpha,\beta)$ physics (RCL/EJP).

Sources

- Spontaneous fission (JSH),
- Multiple-source particle types (JSH/MTS),
- Repeated structures source-path improvement (LLC/JSH),
- Positron sources (HGH),
- Sources on cylindrical surfaces (GWM/JSH),
- Source particles that may be specified by character descriptors (JSH), and
- translated sources with dependence (GWM).

Tallies

- Pulse-height tallies (PHTs) with variance reduction (JSH/GWM),
- Default dose functions (LSW/JSH),
- Pulse-height light tally with anticoincidence: FT8 PHL (GWM),
- Coincidence capture tally: FT8 CAP (MTS/SJT/DRM/JSH),
- Residual nuclei tally: FT8 RES (JSH),
- Lattice tally speedup by orders of magnitude (GWM),
- Proton reaction multipliers with FM cards (JSH),
- Photonuclear reaction multipliers with FM cards (JSH/GWM),
- Expanded radiography tally specification (JSH), and
- Cosine bins that may be specified in degrees and for F2 tallies (JSH).

Other Input File Extensions

- Logarithmic interpolation on input cards (JSH),
- Auxiliary input files (JSH),
- HISTP file size control (LSW),
- DXTRAN improvements (GWM), and
- PTRAC file for all particles and for coincidence counting (MTS/JSH/GWM).

Graphics

- Mesh tallies (tally grid superimposed over geometry) plotted within MCNPX (JSH/GWM);
- Two-dimensional (2D) color tally contour plots of lattice and radiography tallies (GWM);

- Enhanced color geometry plots (GWM/JSH);
- Geometry plot of WWG superimposed mesh (JSH);
- i,j,k lattice indexing in geometry plots (JSH);
- Proton and photonuclear cross-section plots (JSH); and
- Pause command for tally and cross-section plots (JSH).

Parallel Processing

- Distributed memory multiprocessing for all particles and energies (GWM),
- Message passing interface (MPI) multiprocessing (JL/GWM), and
- Significant speedup of criticality problems run with MPI (GWM/NAC).

Compiling, Configuration, and Installation

- FORTRAN90 modularity and dynamic memory allocation (GWM);
- F90 autoconfiguration (TLR/HWE);
- 64-bit integer support (GWM); and
- NAG/IBM/INTEL compiler extensions for Unix, Linux, and Windows (GWM).

1.2. Guarantee

MCNPX is guaranteed. We are so confident of the quality of MCNPX that we will pay \$20 or €20 to the first person finding anything that does not meet or exceed the capabilities of MCNPX 2.3.0 and MCNP4C3. We also will pay a brand new \$2 bill for any error in MCNPX that has been inherited from its constituent codes.*

MCNPX is a better quality code than MCNP4C3.† First, it corrects many MCNP4C3 problems. Second, cash awards have been earned less frequently with MCNPX than with MCNP4C3 and its predecessors, and most of those awards are for problems carrying over from older code versions; very few have been put into the new MCNPX versions. A list of winners is available at <http://mcnpx.lanl.gov/>. MCNPX bugs are described in the newsletter for each MCNPX version.

1.3. Availability

MCNPX 2.5.0 is available from the Radiation Safety Information and Computational Center (RSICC) in Oak Ridge, Tennessee, USA, at <http://www-rsicc.ornl.gov/>. MCNPX 2.5.0 also is expected to be available from the Organization for Economic Cooperation and Development/Nuclear Energy Agency (OECD/NEA) Data Bank in Paris, France, at <http://www.nea.fr/>.

* Cash Award Fine Print: Offer is subject to cancellation or modification without notice. A bug is defined as an error in the source code that we choose to correct. We make awards for even the most trivial or insignificant problems but not for proposed code enhancements or proposed extended capabilities. Awards are given only to the first MCNPX user reporting a problem. Reported problems must be reproducible, and awards are paid when the correction is integrated into a forthcoming MCNPX version. We believe that MCNPX and its predecessor codes are the most error-free and robust Monte Carlo radiation transport capabilities, and we back them with a cash guarantee.

† J. F. Briesmeister, ed., “MCNP—A General Monte Carlo N-Particle Transport Code—Version 4C,” Los Alamos National Laboratory report LA-13709-M (April 2000).

An essential part of the MCNPX software quality assurance plan is the beta test program. Before a code version goes to RSICC or OECD/NEA, it is made available to more than 1600 MCNPX beta testers worldwide. MCNPX beta test versions are available to authorized beta testers on the MCNPX website at <http://mcnpx.lanl.gov/>. Participants in MCNPX workshops automatically become MCNPX beta testers (<http://mcnpxworkshops.com/>). In special cases, others may also obtain beta test access by contacting mcnpx@lanl.gov.

All beta test, RSICC, and OECD/NEA versions of MCNPX are guaranteed with cash awards.

2.0. PHYSICS EXTENSIONS

The following physics capability extensions are available and are controlled by the input cards listed in parentheses:

- Seamless transport of 34-particle types at nearly all energies by mixing and matching of nuclear data table and model physics (PHYS:N, PHYS:H, MX);
- Extension of neutron model physics below 20 MeV (PHYS:N, PHYS:H, PHYS:x);
- Fission multiplicity (PHYS:N, FMULT);
- Light-ion recoil (PHYS:N, PHYS:H);
- Photonuclear model physics (PHYS:P);
- Photon Doppler broadening from MCNP5 (PHYS:P);
- Inline generation of double differential cross sections and residual nuclei (LCA);
- CEM2k physics (LCA);
- INCL4/ABLA physics models (LCA, LEA, LCC);
- Improved $S(\alpha, \beta)$ physics (MT); and
- User specification of fission multiplicity constants (FMULT).

In the following descriptions of input cards, **bold face type** is used to highlight extensions from earlier MCNP or MCNPX input.

2.1. Neutrons: PHYS:N

PHYS:N *EMAX EAN IUNR DNB **TABL FISM RECL***

EMAX = upper energy limit (default = 100 MeV).

Note: EMAX must be higher than the highest energy in the problem or the physics is *wrong*. However, setting EMAX too high causes excessively coarse energy binning of model physics, which is inaccurate. For problems with energies above 100 MeV, EMAX should be chosen carefully; the default is appropriate for problems with energies below 100 MeV.

EAN = analog capture below *EAN*; implicit capture above *EAN* (default = 0 MeV).

IUNR = unresolved resonance range probability table treatment.

= 0/1 = on/off (default = 0) when unresolved data are available.

- DNB*** = delayed neutrons from fission.
 -1 = analog production of delayed neutrons from fission (default).
 0 = treat prompt and delayed neutrons as prompt.
 n = biased production: produce up to n delayed neutrons per fission ($n > 0$ disallowed in KCODE).
- TABL*** = use data tables below *TABL*, physics models above *TABL*.
 = -1 (default) (mix and match). When tables are available, use them up to their upper limit and use the physics models above.
- FISM*** = fission multiplicity.
 = 0 (default) MCNP treatment. The number of neutrons per fission is the integer above or below ν . If $\nu = 2.7$, then the number of neutrons will be two 30% of the time and three 70% of the time.
 = FWHM: sample Gaussian distribution with full-width half-maximum of FWHM about ν .
 = -1: sample Gaussian distribution with FWHM appropriate for fissioning nuclide (recommended).
- RECL*** = 0 (default) no light-ion recoil.
 ≥ 0 : light ion recoil. Produce $0 \leq RECL \leq 1$ light ions (h, d, t, s, a) at each elastic scatter with light nuclei (H, D, T, ^3He , ^4He). The ionization potential is accounted for, and the proper two-body kinematics is used (with neutron free-gas thermal treatment if appropriate) to bank the created particles with the proper energy and angle. *MODE n h d t s a . . .* is required to produce light ions h, d, t, s, a . *CUT:x 2J 0* for $x = h, d, t, s, a$ is recommended so that the low-energy recoil ions produced are not killed by energy cutoff.

2.1.1. Mix and Match (*TABL*)

The *TABL* entry on the PHYS:N and PHYS:H cards controls mix and match. If the energy, E , is greater than *TABL*, physics models will be used above $E = TABL$. Physics models can be used at any energy, even below 20 MeV, although physics models are often poor below 100 to 200 MeV. If *tabl* = -1, then mix and match is used and the data tables are used for their full energy range, when available, for each nuclide, even if other nuclides in the problem do not have data tables available in that energy range. The MCNPX mix-and match-capability is illustrated in Fig. 1.

Two nuclides are present in this example: oxygen and uranium. The oxygen data table ranges from 0 to 150 MeV; the uranium data table ranges from 0 to 20 MeV. If *TABL* = 20, then nuclear data tables are used below 20 MeV and physics models above; the superior table data for oxygen between 20 to 150 MeV are ignored. If *TABL* = 150, then nuclear data tables are used below 150 MeV and physics models above; the values for uranium at 20 MeV are used (incorrectly) in the range of 20 to 150 MeV. However, if *TABL* = -1 (default), mix and match is used: both oxygen and uranium use the table data where they exist and physics models above the maximum energy.

See the discussion of mix and match for the MX card in Section 2.5.



Fig. 1. Mix and match.

2.1.2. Fission Multiplicity (FISM)

Fission multiplicity is the number of neutrons produced in a fission reaction. The nuclear data tables provide the average number fission neutrons, ν , per fission. The default MCNPX treatment is the MCNP treatment: the number of neutrons per fission is the integer above or below ν . If $\nu = 2.7$, then the number of neutrons will be two 30% of the time and three 70% of the time. If the sixth entry, *FISM*, on the PHYS;N card is positive, then ν is sampled from a Gaussian distribution. The full-width at half-maximum (FWHM) of the Gaussian distribution is obtained from the table in Section 2.10. For induced fission, the average value of ν generally comes from the nuclear data library and is a function of the incident neutron energy. For spontaneous fission sources, the fission multiplicity is sampled from a cumulative distribution when available or sampled from a Gaussian distribution when unavailable. The values of the FWHM and spontaneous fission ν may be overridden using an **FMULT** card (Section 2.10).

When a Gaussian distribution is used, the average number of fission neutrons becomes biased above its true value. The high value of ν occurs because ν can have sampled values between $\pm\infty$, and when the negative values of ν are sampled they are set to zero, causing a slightly high bias. The negative Gaussian bias for fission multiplicity has a small correction to preserve the average number of neutrons per fission. The following options are available for the sampling of fission multiplicity*:

* John S. Hendricks, "Monte Carlo Sampling of Fission Multiplicity," Los Alamos National Laboratory report LA-UR-04-6967, submitted to Monte Carlo 2005, Chattanooga, Tennessee (April 17–21, 2005).

PHYS:N 5J *FISM* ,

where

FISM = 0: no fission multiplicity: MCNP method—sample ν from nearest integer, which preserves the first moment but gives incorrect multiplicity;
 = 1: correct sampled ν to preserve average multiplicity (recommended);
 = 2: preserve multiplicity by increasing ν threshold.
 = 3: sample Gaussian distribution without correction;
 = 4: MCNP method in presence of spontaneous fission or FMULT card.

Defaults: If an **FMULT** card is present or if a spontaneous fission source is used (par = sf on SDEF card), then the default is *FISM* = 1; otherwise, the default is *FISM* = 0.

If *FISM* = -1 (MCNPX 2.5.E specification), it is changed to +1 for backward compatibility. To specify a width for fission multiplicity (*FISM* > 0 in MCNPX 2.5.E), the **FMULT** card must be used.

The fission multiplicity—both the number of fission neutrons and the moments of the distributions, are printed in Print Table 117 (Section 3.3.3).

2.1.3. Light-Ion Recoil (RECL)

MCNPX can produce and track ions created by elastic recoil from neutrons or protons. Neutrons and protons undergoing elastic scatter with light nuclei (H, D, T, ³He, and ⁴He) can create ions (protons, deuterons, tritons, ³He, and α) that are banked for subsequent transport.

Figure 2 shows the energy-angle production of alphas created from 15-MeV neutrons striking ⁴He. Note that in the forward bin, cosine $0.8 < \mu < 1$, the α energy goes up to the theoretical maximum of 9.6 MeV. The theoretical maxima in the other cosine bins (0.8, 0.6, 0.4, and 0.2) are 6.144, 3.456, 1.536, and 0.384.

The input file for this example is as follows.

```
Test of light ion recoil
1 1 1e-5 -1
2 0 1

1 so 1.e-5

mode n a
imp:n,a 1 0
phys:n 6j 1
sdef erg=15
print -161 -162
tmp1 1e-20 0
fcl:n 1 0
m1 2004 .2
cut:a j 0
nps 1000000
f51:a 1
e51 .1 100log 20
```

```
c51 -.8 8i 1 t
fq51 e c
```

The plot commands to produce Fig. 2 are presented in the following plot command file.

```
rmct lir.m tal 51 xlim .1 15 loglog &
title 1 "Light-Ion Recoil: 15 MeV Neutrons on 4He" &
title 2 "Alpha Energy vs Cosine" &
fix c 11 label 1 "cos total" cop fix c 6 label 2 "cos -1-.2" &
cop fix c 7 label 3 "cos .2-.4" cop fix c 8 label 4 "cos .4-.6" &
cop fix c 9 label 5 "cos .6-.8" cop fix c 10 label 6 "cos .8-1."
```

2.2. Photons: PHYS:P

PHYS:P *EMCPF* *IDES* *NOCOH* *ISPN* ***NODOP*** ,

where

EMCPF = upper energy for detailed physics (default = 1 MeV);
IDES = generate electrons by mode E or thick-target-bremsstrahlung
 (default = 0 = on);
NOCOH = coherent (Thomson) scattering (default = 0 = on);
ISPN = -1/0/1 = analog/off/biased. The bias causes a photonuclear event at each
 photoatomic event. (default = 0 = off); and
NODOP = 0/1 = on/off Doppler energy broadening. (default = 1 = off).

2.2.1. Photonuclear Model Physics (ISPN)

Photonuclear physics models enable (γ,n) and other photonuclear reactions when photonuclear data tables are unavailable. When some photonuclear data tables are available, MCNPX will mix and match, using tables when available and physics models when no tables are available. The user interface is not changed; the user simply gets the latest *gdr.dat* file from the MCNPX source file, *src/DATA/CEM/gdr.dat*. The threshold for photonuclear reactions is 1 MeV.

The MCNPX photonuclear physics model modifications adjust the photofission cross sections in CEM by the ratio of fission and neutron evaporation-level density parameters (*wam*). For selected isotopes (thorium, uranium, and plutonium), a list of energy-dependent *wam* parameters was generated by matching the fissility of the BOFOD photonuclear cross-section data. The lists are entered into the code as data statements in subroutine *set_wam*. This subroutine provides a *wam* parameter for a requested nuclide "IZA" at an incident photon energy of "t0mev" interpolating between two tabulated values. If data for a requested nuclide are not available, *wam* is returned as 0.0. We hope to provide *wam* parameters for more isotopes in the future. Also, an improved fit of photoabsorption cross sections in the updated CEM2k *pnxs.F* routine occurs based on experimental data from Muccifora, Bianchi, Brookes, Michalowski, and Chollet.*

* Franz Gallmeier, private communication, April 2004.

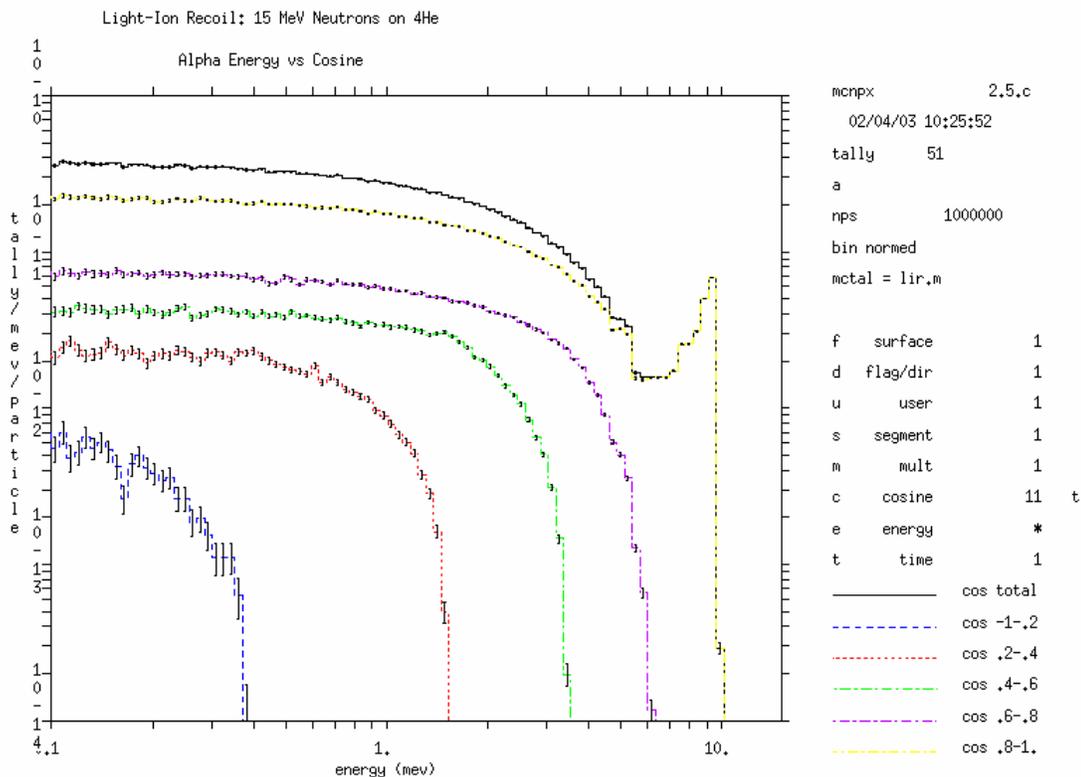


Fig. 2. Light-ion recoil.

Photonuclear models are designed to work with the CEM2k physics package and are fragile or may not work with other packages.

2.2.2. Photon Doppler Broadening (NODOP)

The MCNP5 photon Doppler broadening capability* developed by Avneet Sood is available in MCNPX. Unlike MCNP5, the default is “off” (PHYS:P 4j 1) because the effect is small but time consuming. When photon Doppler broadening is turned on (NODOP = 0), it has no effect unless photon Doppler broadening momentum profile data are available in the photon library. These data are available in the MCPLIB03 and MCPLIB04 photon libraries with ZAIID identifiers .03p and .04p.

The electron binding effect on a scattered photon’s energy distribution appears as a broadening of the energy spectrum due to the precollision momentum of the electron. The effect applies to incoherent scatter (Compton scatter). The scattered energy of a Doppler-broadened photon is calculated by selecting an orbital shell, sampling the projected momentum from the Compton profile, and then calculating the scattered photon energy.

* X-5 Monte Carlo Team, “MCNP—A General Monte Carlo N-Particle Transport Code, Version 5, Volume II: User’s Guide,” Los Alamos National Laboratory report LA-CP-03-0245 (April 24, 2003), pp. 2–59.

Two research notes on photon Doppler broadening are available on the MCNPX web site, <http://mcnpx.lanl.gov/documents/>. The following is quoted from one of these research notes (X-5:AS-02-16).

Incoherent scattering of an incident photon can occur with a bound electron in a shell of a material and will generate a Compton electron and a scattered photon. The electron binding effects become important when the incident photon energy is near a few hundred keV. The result of the binding effects on the angle and energy of the scattered photon must be taken into account for accurate simulation of low-energy photon transport. The effect of the bound electron on the scattered photon's angular distribution appears as a reduction in the total scattering cross section in the forward direction. MCNP currently accounts for the electron binding effects on the angular distribution of the scattered photon by modifying the Klein-Nishina differential cross section with a form factor. The electron binding effect on the scattered photon's energy distribution appears as a broadening of the energy spectrum due to the precollision momentum of the electron. This effect on the energy distribution of the incoherently scattered photon is called Doppler broadening.

2.3. Protons: PHYS:H

PHYS:H *EMAX EAN TABL J ISTRG J RECL* ,

where

EMAX = upper energy limit (default = 100 MeV).

Note: *EMAX* must be higher than the highest energy in the problem or the physics is *wrong*. However, setting *EMAX* too high causes excessively coarse energy binning of model physics, which is inaccurate. For problems with energies above 100 MeV, *EMAX* should be chosen carefully; the default is satisfactory for problems with energies below 100 MeV.

EAN = analog capture below *EAN*; implicit capture above *EAN* (default = 0 MeV)

TABL = use data tables below *TABL*; physics models above *TABL*
= -1 (default) (mix and match). If tables are available, use them up to the upper energy limit and use physics models above

J = jump (unused)

ISTRG = charged particle straggling control
= 0 Vavilov (default, best)
= 1 continuous slowing down approximation
= -1 old MCNPX 2.2.4 method

J = jump (unused)

RECL = light-ion recoil. Produce $0 < RECL < 1$ light ions (*h, d, t, s, a*) at each elastic scatter with light nuclei (H, D, T, ³He, ⁴He). The ionization potential is accounted for, and the proper two-body kinematics is used to bank the created particles with the proper energy and angle. MODE h

d t s a ... is required to produce light ions (h, d, t, s, a). *CUT:x 2J 0* for x = h, d, t, s, a is recommended so that the low-energy recoil ions produced are not killed by energy cutoff. Note that protons colliding with hydrogen to produce more protons can produce an overwhelming number of protons; caution is required, and *RECL < 1* may be needed.

See the definitions of *TABL* and *RECL* in the description of the neutron physics card, *PHYS:N*, above.

2.4. Charged Particles: *PHYS:x*

PHYS:x EMAX 3J ISTRG ,

where

EMAX = upper energy limit (default = 100 MeV).

Note: *EMAX* must be higher than the highest energy in the problem or the physics *is wrong*. However, setting *EMAX* too high causes excessively coarse energy binning of model physics, which is inaccurate. For problems with energies above 100 MeV, *EMAX* should be chosen carefully; the default is satisfactory for problems with energies below 100 MeV.

J = jump (unused)

ISTRG = charged particle straggling control

= 0 Vavilov or Prael's straggling model, which is an energy correction addressing stopping powers. (default, best)

= 1 continuous slowing down ionization model

= -1 old MCNPX 2.2.4 method

2.5. Mix-and-Match Nuclide Replacement: *MX*

The *MX* card enables materials substitution for different particle types. This card is an extension of, and replacement for, the *MPN* card for photonuclear data

MXn:p zaid1 zaid2 ... ,

where

n = material number of an *Mn* card that **MUST** precede the *MXn* card,

p = particle type (n, p, h), and

zaidn = ZA of replacement nuclide for the *n*th nuclide on the *Mn* card.

Only particle types n (neutron), p (photonuclear), and h (proton) are allowed on the *MX* card. No substitutions are allowed for photoatomic (p) and electron (e) data because those data sets are complete. The *MXn:P* card is an exact replacement of the *MPNn* card and specified photonuclear nuclide substitutions (library type u). *zaidn* = 0 is allowed on *MXn:P* (photonuclear substitution) to specify no photonuclear data for a specific photoatomic reaction. *zaidn* = model is allowed on

the MXn:N and MXn:H (neutron and proton substitution) to allow models to be mixed with tabular data. As an example, consider the following input file.

```

mode n h p
m1          1002 1      1003.6 1      6012 1      20040 1      nlib .24c
mx1:n       j          model      6000      20000
mx1:h       model     1001      j          j
mpn1        6012      0          j          j
    
```

MCNPX will issue the following warnings.

```

warning. MPNn will soon be obsolete. Use MXn:p instead.
warning. photonuclear za = 6012 different from nuclear za = 1002
warning. photonuclear za = 0 different from nuclear za = 1003
    
```

Models will be used for neutron tritium and proton deuterium. The MPN card still works but has a warning. The mixing and matching is summarized in Print Table 101:

particles and energy limits print table 101

Particle Type	Particle Cutoff Energy	Maximum Particle Energy	Smallest Table Maximum	Largest Table Maximum	Always Use Table Below	Always Use Model Above
1 n neutron	0.0000E+00	1.0000E+37	1.5000E+02	1.5000E+02	0.0000E+00	1.5000E+02
2 p photon	1.0000E-03	1.0000E+02	1.0000E+05	1.0000E+05	1.0000E+05	1.0000E+05
9 h proton	1.0000E+00	1.0000E+02	1.5000E+02	1.5000E+02	0.0000E+00	1.5000E+02

The MCNPX mix-and-match capability* enables mixing and matching of physics models and data tables. It is possible to specify some nuclides with models and other nuclides with data tables (isotope “mixing”). It is also possible to use data tables up to their maximum energy value and then use models above that energy, even when the maximum table energy differs from nuclide to nuclide (“energy matching”).

As an example, consider protons interacting with a bismuth-germanium particle detector (BGO). Because the present LA-150 nuclear data libraries† do not include germanium, it was previously possible to use physics models alone for all nuclides in the entire problem. With the mix-and-match capability, bismuth and oxygen can be modeled with the more accurate nuclear data tables, whereas germanium uses a physics model.

* John S. Hendricks, “MCNPX Model/Table Comparison,” Los Alamos National Laboratory report LA-14030 (March 2003).

† M. B. Chadwick, P. G. Young, S. Chiba, S. C. Frankle, G. M. Hale, H. G. Hughes, A. J. Kongin, R. C. Little, R. E. MacFarlane, R. E. Prael, and L. S. Waters, “Cross Section Evaluations to 150 MeV for Accelerator-Driven Systems and Implementation in MCNPX,” Nuclear Science and Engineering **131**: 3 (March 1999), 293.

As another example, consider a neutron problem with deuterium and tritium. The available deuterium library goes up to 150 MeV, but the tritium library goes up to only 20 MeV. Previously, either neutron physics models above 20 MeV (neglecting the deuterium table data up to 150 MeV) or nuclear data tables below 150 MeV (using the 20-MeV tritium data throughout the entire 20- to 150-MeV range) had to be used. With the mix-and-match capability, deuterium uses tables up to 150 MeV and uses physics models above 150 MeV; tritium uses data tables up to 20 MeV and uses physics models above 20 MeV.

Figure 3 shows an example of the energy-matching capability. The 100-MeV neutrons are incident on an 8.433-cm-long, 3.932-cm-radius BGO crystal. The crystal contains 21% bismuth, 16% germanium, and 63% oxygen. Currently, no germanium libraries are available. The solid line represents flux in the crystal with the full mix-and-match capability, which uses all libraries up to their energy limits and physics models above those limits and for germanium. The dashed-line calculation uses the old method of substituting arsenic for the missing germanium library, using the libraries up to 20 MeV and using physics models above. The dotted line uses bismuth and oxygen libraries up to their limits of 150 MeV; the arsenic library is used up to its limit of 20 MeV, and then the 20-MeV data are used from 20 to 150 MeV; above 150 MeV, physics models are used for all three nuclides. This last option is least desirable but often was used in past code versions to take advantage of the 150-MeV libraries, even though many data libraries go only to 20 MeV.

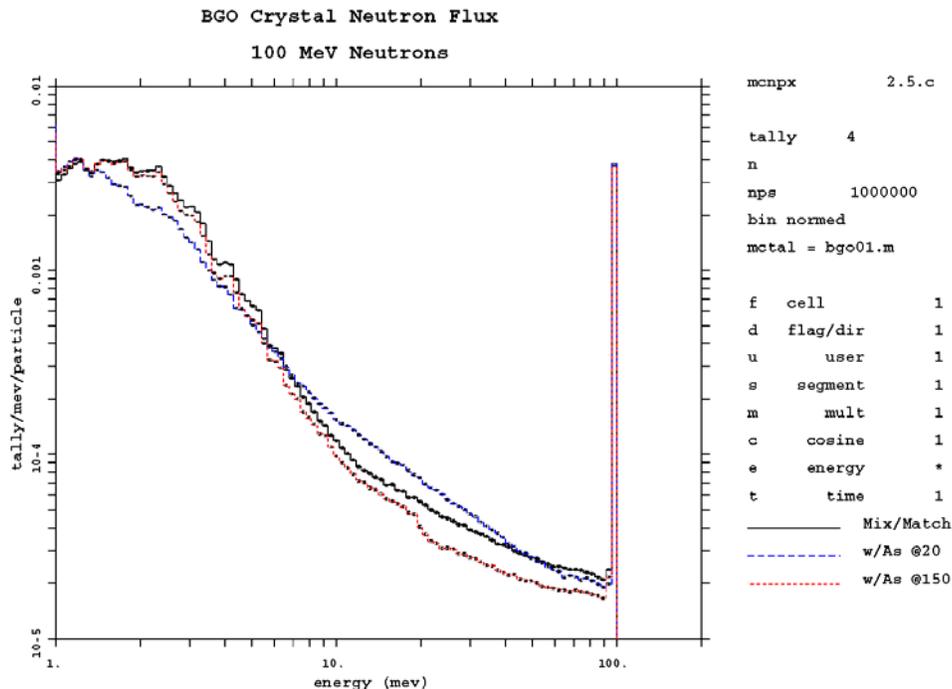


Fig. 3. Comparison of different germanium library and model options.

The mix-and-match capability is particularly useful for photonuclear calculations because few photonuclear data tables are available currently. Libraries are used when available, and models are used otherwise. Note that photonuclear physics is modeled with the CEM2k model, regardless of whether CEM is used for other particles.

Different nuclides can be substituted for different particle types. For example, natural carbon and calcium can be used for neutrons, whereas ^{12}C and ^{40}Ca can be used for protons and photonuclear reactions.

2.6. Physics Models: LCA

LCA *IELAS IPREQ IEXISA ICHOIC JCOUL NEXITE NPIDK NOACT ICEM* ,

where

<i>IELAS</i>	= 0 / 1 / 2 (default) = no/neutron only/neutron and proton elastic scattering
<i>IPREQ</i>	= 0 = no preequilibrium model will be used = 1 (default) = use preequilibrium model after intranuclear cascade = 2 = select IPREQ = 1 and IPREQ = 3 randomly if IEXISA = 0 = 3 = use preequilibrium model instead of the intranuclear cascade if IEXISA = 0
<i>IEXISA</i>	= 0 = do not use ISABEL intranuclear cascade (default if ICEM = 2 = INCL4) = 1 (default) = use Bertini for nucleons and pions and ISABEL for other particles = 2 = use ISABEL for all particles
<i>ICHOIC</i>	= ISABEL model control (0023 = default)
<i>JCOUL</i>	= 0 / 1 (default) = no/yes Coulomb barrier for incident charged particles
<i>NEXITE</i>	= 1 (default) / 2 = subtract nuclear recoil energy to get excitation energy
<i>NPIDK</i>	= 0 (default) / 1 = force pi- nuclear capture below pi- energy cutoff
<i>NOACT</i>	= -2 = source particles immediately collide; all progeny escape. Used to compute double differential cross sections and residual nuclei. = -1 = nuclear interactions of source particles only—transport and slowing down are off. Used to compute double-differential cross sections with XSEX code. = 0 = turn off all nonelastic reactions = 1 (default) = normal transport = 2 = attenuation mode—transport primary source particles without nonelastic
<i>ICEM</i>	= 0 (default) = Use Bertini or ISABEL model determined by IEXISA = 1 = use CEM2k model = 2 = use INCL4 model (default ABLA fission-evaporation)

2.6.1. Inline Generation of Double Differential Cross Sections and Residual Nuclei

The *NOACT* option on the LCA card enables MCNPX to calculate a single interaction in the physics model region. If the eighth entry on the LCA card is -2,

LCA 7J -2 ,

then the source particle immediately will have a collision and all subsequent particles will escape. That is, LCA(8) = -2 causes the source particle to have a distance to collision of zero, and all subsequent tracks have a distance to collision of infinity.

The double differential cross sections and distributions of residual nuclei for a single nuclear interaction thus may be calculated directly in MCNPX. Tallying of the residual nuclei is discussed later in the FT8 RES tally description (see Section 4.9). Tallying of the differential cross section can be done with standard F1 surface tallies, as shown in the following example. The input file models a 1.2-GeV proton source having a single collision with ²⁰⁸Pb.

```
Test of p(1.2GeV)+Pb(208)
1 1 -11. -1 imp:h 1
2 0      1 imp:h 0

1 so .01

mode h n
sdef par h erg=1200 vec 0 0 1 dir 1
m1 82208 1
phys:h 1300 j 0
phys:n 1300 3j 0
nps 10000
fc1 *** neutron angle spectra tally ***
f1:n 1
ft1 frv 0 0 1
fq1 e c
*c1 167.5 9i 17.5 0 T
e1 1 50log 1300 T
lca 2 1 1 23 1 1 0 -2 0
```

The differential cross section for neutron production is tallied in the F1 current tally with energy and time bins. This tally is simply the neutrons that are created from the single proton collision with lead and then escape. These data may be plotted with MCNPX using the tally plotter and then following execute line command

MCNPX Z ,

where the command file, COM91, is

```
rmctal=mct191
file all loglog xlim 1 1300 ylim 1e-6 1 &
fix c 13 cop fix c 1 cop fix c 6 cop fix c 12
```

In Fig. 4, the first line (solid black) is the energy spectrum over all angles, the second (blue dashed) is the 180° output, the third (red dotted) is the 90° output, and the fourth (green broken) is the 0° output.

2.6.2. CEM2k Physics Model (ICEM)

The MCNPX CEM physics model has been upgraded from CEM95 to CEM2k.* It still is controlled solely by the ninth entry, ICEM, on the LCA card. The model assumes that reactions occur in three stages. The first stage is the IntraNuclear Cascade (INC), in which primary particles can be rescattered, thus producing secondary particles several times before absorption by or escape from the nucleus. The excited residual nucleus that remains after the cascade determines the particle-hole configuration, which is the starting point for the preequilibrium stage of the reaction. The subsequent relaxation of the nuclear excitation is treated in terms of an improved modified exciton model of preequilibrium decay, followed by the equilibrium evaporative final stage of the reaction, which is competing with the fission and Fermi-breakup channels.

CEM2k incorporates the latest approximations for the elementary cross sections used in the cascade, using more precise values for nuclear masses and pairing energies, corrected systematics for the level-density parameters, and several other refinements. Improved algorithms decrease the computing time by up to a factor of 6 for heavy targets. Other improvements were

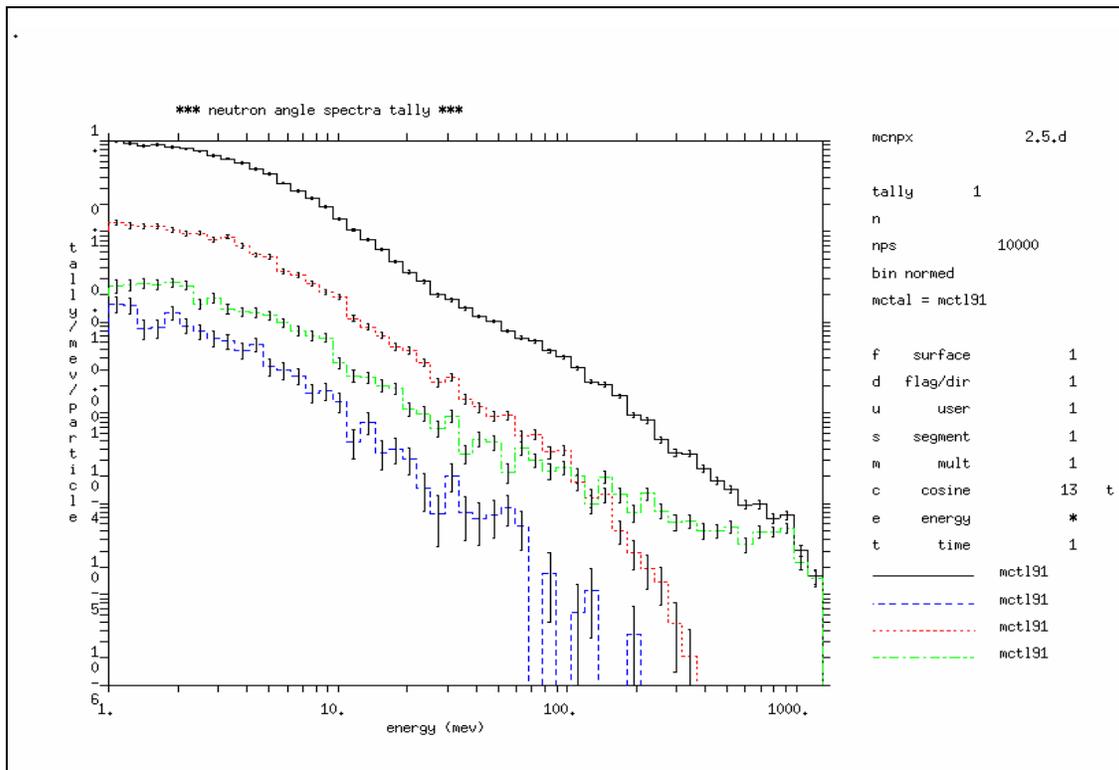


Fig. 4. Differential cross sections at all angles, 180°, 90°, and 0°, for 1.3-GeV protons on $^{208}_{82}\text{Pb}$.

* S. G. Mashnik and A. J. Sierk, "Recent Developments of the Cascade-Exciton Model of Nuclear Reactions," Los Alamos National Laboratory report LA-UR-01-5390, and International Conference on Nuclear Data for Science and Technology, Tsukuba, Japan (October 7–12, 2001).

motivated by recent measured data on isotope production from Gesellschaft für Schwerionenforschung (GSI) (mbH, Darmstadt, Germany) experiments. Compared with earlier versions, CEM2k has a longer cascade state, less preequilibrium emission, and less evaporation from more highly excited compound nuclei. CEM2k also has better models of neutron, radionuclide, and gas production in accelerator-transmutation-of-waste spallation targets.

A photonuclear physics package has been added to CEM2k by Franz Gallmeier [Oak Ridge National Laboratory (ORNL)] for photon energies from 8 MeV to about 2 GeV and includes the Giant Dipole and Quasi-Deuteron resonances. These photonuclear physics models compliment existing photonuclear data evaluations in that they may be used for nuclides where no tabular data exist. Also, they may be used for tabular-data nuclides above the 150-MeV upper-energy boundary of the tables.

2.6.3. INCL4/ABLA (Cugnon/Schmidt) Physics Models (ICEM)

The IntraNuclear Cascade, Liege (INCL4) and ABLA fission-evaporation models are available in MCNPX. They are controlled by the LCA, LCC, and LEA input cards:

LCA(9) = 2 INCL4 model (sets LCA(3) = *IEXISA* = 0)
 LEA(7) = 2 ABLA fission evaporation
 LCC = control parameters for INCL4

INCL4 and ABLA may be used in various combinations with other physics models.

Bertini/Dresner:	LCA 2 1 1 23 1 1 0 1 0	\$ MCNPX Default: Bertini
	LEA 1 4 1 0 1 0 0 1	\$ MCNPX Default: Dresner
CEM2k	LCA 8J 1	\$ CEM2k works alone
ISABEL/Dresner	LCA 2J 2	\$ ISABEL
Bertini/ABLA	LEA 6J 2	\$ ABLA
ISABEL/ABLA	LCA 2J 2	\$ ISABEL
	LEA 6J 2	\$ ABLA
INCL4/Dresner	LCA 8J 2	\$ INCL4
INCL4/ABLA	LCA 8J 2	\$ INCL4
	LEA 6J 2	\$ ABLA

These combinations also may be shown in the following table.

	LCA(3) <i>IEXISA</i>	LCA(9) <i>ICEM</i>	LEA(7) <i>IEVAP</i>
Bertini/Dresner	1	0	0
ISABEL/Dresner	2	0	0
Bertini/ABLA	1	0	2
ISABEL/ABLA	2	0	2
CEM2k	-	1	-
INCL4/Dresner	0	2	0
INCL4/ABLA	0	2	2

The INCL4 model is based largely on the work of Joseph Cugnon at the University of Liege in Liege, Belgium. This model generally is coupled with the ABLA fission-evaporation model that

was developed principally by Karl-Heinz Schmidt at GSI. Its integration into MCNPX has been done principally by Jean-Christophe David at Commissariat à l'Energie Atomique-Saclay, France.

INCL4 and ABLA are intended for use in the 200-MeV to 2-GeV energy range. Only two free parameters exist in INCL4: the potential depth V_0 (default = 45 MeV) and the overall factor f_{stop} (default = 1.0). These parameters are controlled by the LCC card.

The INCL4 model, in its present implementation, is much slower than the Bertini and CEM2k models.

2.7. INCL4 Options: LCC

LCC *STINCL V0INCL*

The LCC card specifies options for the INCL4 model and the ABLA fission-evaporation model. INCL is invoked by setting the ninth LCA card entry to 2, and ABLA is invoked by setting the seventh LEA card entry, IEVAP, to 2. The LCC card entries are

- (1) *STINCL* rescaling factor of the cascade duration (default = 1)
- (2) *V0INCL* potential depth (default = 45 MeV)

2.8. ABLA Fission-Evaporation Model: LEA

LEA *IPHT ICC NOBALC NOBALE IFBRK ILVDEN IEVAP NOFIS* ,

where

IPHT = 0 / 1 (default) = no/yes generate de-excitation photons
ICC = 0 / 1 / 2 / 3 / 4 (default) = continuum/Troubetzkoy/intermediate/
 spin-dependent/full PHT physics model.
NOBALC = 0 / 1 (default) no/yes—turn off mass-energy balancing in cascade
NOBALE = 0 (default) / 1 = mass-energy balancing in evaporation
IFBRK = 0 / 1 (default) = Fermi breakup model nuclide range
ILVDEN = -1 / 0 (default) / 1 = HETC/Gilbert/Julich—level density model
IEVAP = 0 (default) / 1 / 2 = RAL/ORNL/ABLA fission-evaporation model
NOFIS = 0 / 1 (default) = suppress/allow - fission

2.9. Improved $S(\alpha,\beta)$ Treatment: MT

The $S(\alpha,\beta)$ thermal neutron treatment user interface is unchanged, but the underlying secondary energy treatment is improved. In many cases, the $S(\alpha,\beta)$ thermal neutron treatment uses discrete energies instead of 32-equiprobable bin histogram energies. The result is nonphysical spikes in the thermal neutron spectrum that are smoothed out by an algorithm provided by Bob Little and Eric Pitcher of Los Alamos National Laboratory. MCNPX still can track the old algorithm by setting $DBCN(20) = 1$.

2.10. User Specification of Multiplicity Constants: FMULT

The FMULT card enables users to override or add additional fission multiplicity data as

FMULT *Z A I D* [*keyword = values*] ,

where the keywords are

Z A I D = nuclide for which data are entered.
SFnu = average ν for sampling spontaneous fission multiplicity from a Gaussian distribution with *Width*; or
 = cumulative probability of spontaneous fission multiplicity.
SFnu is used for spontaneous fission only; for induced fission, ν is taken from the nuclear data library at the energy of the incident neutron.
Width = Gaussian width for sampling ν for both spontaneous and induced fission, ignored for spontaneous fission when *SFnu* is specified as a cumulative probability distribution.
SFYield = spontaneous fission yield (n/s-g)—used for selecting the spontaneous fission nuclide when more than one is present in a material.
Watt = watt energy spectrum parameters a and b for spontaneous fission neutron energy sampling. Induced fission energies are sampled from the nuclear data library.

Z A I D must be specified. Defaults exist only for the most common fission nuclei; these defaults are provided in Print Table 38 of the MCNPX output. *Width* is used for both spontaneous and induced fission; *SFYield* is used only for spontaneous fission. *SFnu* and *Watt* are used only for spontaneous fission; for induced fission, the values are sampled from the nuclear data library.

Examples:

FMULT 98252 *SFYield* = 2.34e12 *SFnu* = .002 .028 .155 .428 .732 .917
 .983 .998 1. *Width* = 1.207 *Watt* = 1.18 1.03419

FMULT 94239 *Watt* = .885247 3.8026 *Width* = 1.14 *SFYield* = .0218 *SFnu* =
 2.16

All values are printed in the MCNPX output file in Print Table 38. The data in Table 1 are the default values in MCNPX, not the values modified with the FMULT cards above. The default values* have been obtained from Brookhaven National Laboratory and other sources modified by Peter Santi and referenced by him.† The spontaneous fission multiplicity table values are printed in Print Table 38 to only three-digit accuracy but are accurate to seven digits in MCNPX.

* John S. Hendricks, “New Spontaneous Fission Data,” Los Alamos National Laboratory internal memorandum D-5:JSH-2005-064 (December 14, 2004).

† P. Santi, D. Beddingford, and D. Mayo, “Revised Prompt Neutron Emission Multiplicity Distributions for 236, 238-Pu,” Los Alamos National Laboratory report LA-UR-04-8040 (December 2004).

N. E. Holden and M. S. Zucker, BNL-NCS-35513-R. IAEA Advisory Group Meeting on Neutron Standard Reference Data, November 12–16, 1984, Geel, Belgium.

Table 1. MCNPX Output File Print Table 38 Displaying Fission Multiplicity Data

lfission multiplicity data.						print table 38									
zaid	width	wattl	watt2	yield	sfnu										
90232	1.079	.800000	4.00000	6.00E-08	2.140										
92232	1.079	.892204	3.72278	1.30E+00	1.710										
92233	1.041	.854803	4.03210	8.60E-04	1.760										
92234	1.079	.771241	4.92449	5.02E-03	1.810										
92235	1.072	.774713	4.85231	2.99E-04	1.860										
92236	1.079	.735166	5.35746	5.49E-03	1.910										
92238	1.230	.648318	6.81057	1.36E-02	0.048	.297	.722	.950	.993	1.00	1.00	1.00	1.00	1.	
93237	1.079	.833438	4.24147	1.14E-04	2.050										
94236	0.000	.000000	0.00000	0.00E+00	0.080	.293	.670	.905	.980	1.00	1.00	1.00	1.00	1.	
94238	1.115	.847833	4.16933	2.59E+03	0.056	.267	.647	.869	.974	1.00	1.00	1.00	1.00	1.	
94239	1.140	.885247	3.80269	2.18E-02	2.160										
94240	1.109	.794930	4.68927	1.02E+03	0.063	.295	.628	.881	.980	.998	1.00	1.00	1.00	1.	
94241	1.079	.842472	4.15150	5.00E-02	2.250										
94242	1.069	.819150	4.36668	1.72E+03	0.068	.297	.631	.879	.979	.997	1.00	1.00	1.00	1.	
95241	1.079	.933020	3.46195	1.18E+00	3.220										
* 96242	1.053	.887353	3.89176	2.10E+07	0.021	.168	.495	.822	.959	.996	.999	1.00	1.00	1.	
96244	1.036	.902523	3.72033	1.08E+07	0.015	.131	.431	.764	.948	.991	1.00	1.00	1.00	1.	
96246	0.000	.000000	0.00000	0.00E+00	0.015	.091	.354	.699	.917	.993	1.00	1.00	1.00	1.	
96248	0.000	.000000	0.00000	0.00E+00	0.007	.066	.287	.638	.892	.982	.998	1.00	1.00	1.	
97249	1.079	.891281	3.79405	1.00E+05	3.400										
98246	0.000	.000000	0.00000	0.00E+00	0.001	.114	.349	.623	.844	.970	1.00	1.00	1.00	1.	
98250	0.000	.000000	0.00000	0.00E+00	0.004	.040	.208	.502	.801	.946	.993	.997	1.00	1.	
98252	1.207	1.180000	1.03419	2.34E+12	0.002	.028	.153	.427	.733	.918	.984	.998	1.00	1.	
98254	0.000	.000000	0.00000	0.00E+00	0.000	.019	.132	.396	.714	.908	.983	.998	1.00	1.	
100257	0.000	.000000	0.00000	0.00E+00	0.021	.073	.190	.390	.652	.853	.959	.993	1.00	1.	
102252	0.000	.000000	0.00000	0.00E+00	0.057	.115	.207	.351	.534	.717	.863	.959	.997	1.	

* = used in problem.

All of the available data are printed when Print Table 38 is turned on by the **PRINT** card. Data actually used are denoted by an *. If any data are overridden by FMULT user input, the user data replaces the default data shown in Print Table 38.

2.10.1. Nuclides without Transport Cross Sections

MCNP(X) does not provide nuclear cross sections for transporting ^{246}Cf , ^{254}Cf , ^{257}Fm , and ^{252}No .

To model spontaneous fission from these nuclides, it is necessary to do the transport either with a physics model or by substituting cross sections. Physics models are not recommended at fission energies. To make a nuclide substitution, the AWTAB and MX cards must be used. For example,

```

M123      100257      1.
AWTAB    100257    257.

```

-
- N. Ensslin, W. C. Harker, M. S. Krick, D. G. Langer, M. M. Pickrell, and J. E. Stewart, "Application Guide to Neutron Multiplicity Counting," Los Alamos National Laboratory report LA-13422-M (1998).
- M. S. Zucker and N. E. Holden, "Californium-252 and ^{238}U Nuclear Parameters of Safeguards Interest," Brookhaven National Laboratory report BNL-34804 (1983).
- N. E. Holden and M.S. Zucker, "Prompt Neutron Multiplicity for the Transplutonium Nuclides," Brookhaven National Laboratory report BNL-NCS-36379. *Proc. Int. Conf. Nucl. Data for Basic and Applied Science*, May 13-17, 1985, Santa Fe, New Mexico (1985).
- D. A. Hicks, J. Ise, Jr., and R. V. Pyle, "Probabilities of Prompt-Neutron Emission from Spontaneous Fission," *Phys. Rev.* **101**, 1016 (1956).
- W. W. T. Crane, G. H. Higgins, and H. R. Bowman, "Average Number of Neutrons per Fission for Several Heavy-Element Nuclides," *Phys. Rev.* **101**, 1804 (1956).
- J. W. Boldeman and M.G. Hines, *Nucl. Sci. Eng.* **91**, 114 (1985).
- B. C. Diven, H. C. Martin, R. F. Taschek, and J. Terrell, "Multiplicities of Fission Neutrons," *Phys. Rev.* **101**, 1012 (1956).

MX123:N 98252.

The AWTAB card provides the atomic weight ratio for ^{257}Fm , which is not provided in the standard MCNP(X) data libraries. The MX123:N card substitutes ^{252}Cf , for which there is neutron cross section data, for the corresponding nuclide (100257) on the M123 materials card.

2.10.2. Nuclides without Multiplicity Data

Fission widths, watt fission spectra parameters, and fission yields are not available for the above nuclides, which do not have transport cross sections: ^{246}Cf , ^{254}Cf , ^{257}Fm , and ^{252}No . They are also not available for ^{246}Pu , ^{246}Cm , ^{248}Cm , and ^{250}Cf . Note that the values for width, watt1, watt2, and yield in print table 38 (above) are all zero for these eight nuclides. To have a spontaneous fission source for these nuclides, an FMULT input file data card is required. For example,

```
FMULT 96246 width = 1.1 watt = .2 4 sfyield 1 .
```

Because the multiplicities are provided as a table with 10 bins, the width is ignored for the spontaneous fission source; however, a value is still required for induced fission. For spontaneous fission, the energy distribution is sampled from the two watt-fission spectra parameters; for induced fission, the energy spectra is chosen from parameters in the nuclear data tables of the transport cross sections. Finally, the spontaneous fission yield must be specified if more than one spontaneous fission source nuclide occurs. The yield is used to determine the relative sampling between spontaneous fission source nuclides. These parameters have no default values; if the FMULT card is missing, a fatal error message is issued:

```
fmult card needed for za = 96246 .
```

3.0. SOURCE FEATURES

Most MCNPX source extensions are controlled by the SDEF card:

- source particles that may be specified by descriptors,
- positron sources,
- spontaneous fission,
- multiple-source-particle types,
- sources on cylindrical surfaces,
- repeated structures source-paths, and
- translated sources with dependence.

3.1. Particle-Type Specification: SDEF

The source particle type may be specified on the SDEF card by either its symbol

SDEF PAR = **h**

or by its number

SDEF PAR = **9** .

3.2. Positron Sources: SDEF

Positron sources may be specified as

SDEF PAR = **-e**

or

SDEF PAR = **-3** .

Note that positron physics in MCNPX, just as with MCNP and the Integrated Tiger Series (ITS), is identical to electron physics, except for positron annihilation. Electrons below the energy cutoff are terminated, whereas positrons below the energy cutoff produce annihilation photons. Also, the positrons have a positive charge and may be tallied using the FT card ELC option.

3.3. Spontaneous Fission Sources: SDEF

The spontaneous fission source can be specified in either of two ways:

SDEF par = **SF** normalize summary and tally information by the number of spontaneous fission neutrons, or

SDEF par = **-SF** normalize summary and tally information by the number of histories (generally the number of spontaneous fissions).

3.3.1. Spontaneous Fission Physics

Eighteen nuclides are available: ^{232}Th , ^{232}U , ^{233}U , ^{234}U , ^{235}U , ^{236}U , ^{238}U , ^{237}Np , ^{238}Pu , ^{239}Pu , ^{240}Pu , ^{241}Pu , ^{242}Pu , ^{241}Am , ^{242}Cm , ^{244}Cm , ^{249}Bk , and ^{252}Cf .

Cells are sampled according to the usual SI and SP distributions. If more than one spontaneous fission nuclide is present in a source cell, the fissioning nuclide will be chosen proportionately to the product of its atom fraction and the spontaneous fission yield for each nuclide. If no spontaneous fission nuclide is found in a specified source cell, the code exits with a *bad trouble* error, “spontaneous fission impossible.”

The number of spontaneous fission neutrons then is sampled. The spontaneous fission multiplicity data from Santi and references cited by him (Section 2.10) are used. The energies are sampled from a Watt spectrum with appropriate spontaneous fission parameters for the selected nuclide. Currently, only the first spontaneous fission neutron from each history is printed. If the spontaneous fission samples a multiplicity of zero—that is, no neutrons for a given spontaneous

fission—then the history is omitted from the first 50 history lists of Print Table 110. The number of source particles is equal to the number of spontaneous fission neutrons, which will be ν times the requested number of source histories on the NPS card.

Fission multiplicity for induced fissions (6h entry, PHYS:N card) automatically is turned on with the default width (FISM = -1 = nuclide dependent). If FISM > 0 on the PHYS:N card, then that value will be used.

3.3.2. Normalization of Summary and Tally Information

The MCNPX spontaneous fission source is different from most other SDEF fixed sources. Let

- N = NPS from the NPS card = the number of source particle histories,
- W = the average source particle weight, and
- ν = the average number of spontaneous fission neutrons per fission.

For most other MCNPX fixed source (SDEF) problems,

- summary table source tracks = N,
- summary table source weight = W, and
- summary tables and tallies are normalized by N.

For the spontaneous fission source, SDEF par = SF ,

- summary table source tracks = $\nu \cdot N$,
- summary table source weight = W, and
- summary tables and tallies are normalized by $\nu \cdot N$.

For the spontaneous fission source, SDEF par = -SF,

- summary table source tracks = $\nu \cdot N$,
- summary table source weight = $\nu \cdot W$, and
- summary tables and tallies are normalized by N.

3.3.3. Fission Multiplicity Output

Multiplicity and moments are printed in Print Table 117 for both spontaneous and spontaneous plus induced fissions.

spontaneous fission source multiplicity and moments.								print table 117
	----- by number -----			----- by weight -----				
	fissions	neutrons	multiplicity fraction	fissions	fission neutrons	multiplicity fraction	error	
nu = 0	697	0	6.97000E-02	3.24005E-02	0.00000E+00	6.97000E-02	0.0373	
nu = 1	2295	2295	2.29500E-01	1.06685E-01	1.06685E-01	2.29500E-01	0.0197	
nu = 2	3261	6522	3.26100E-01	1.51590E-01	3.03180E-01	3.26100E-01	0.0161	
nu = 3	2518	7554	2.51800E-01	1.17051E-01	3.51153E-01	2.51800E-01	0.0187	
nu = 4	1025	4100	1.02500E-01	4.76478E-02	1.90591E-01	1.02500E-01	0.0305	
nu = 5	183	915	1.83000E-02	8.50688E-03	4.25344E-02	1.83000E-02	0.0736	
nu = 6	21	126	2.10000E-03	9.76199E-04	5.85720E-03	2.10000E-03	0.2181	
total	10000	21512	1.00000E+00	4.64857E-01	1.00000E+00	1.00000E+00	0.0073	

factorial moments	by number		by weight	
nu	2.15120E+00	0.0054	2.15120E+00	0.0054
nu(nu-1)/2!	1.91100E+00	0.0116	1.91100E+00	0.0116
nu(nu-1)(nu-2)/3!	8.86800E-01	0.0219	8.86800E-01	0.0219
nu(nu-1) (nu-3)/4!	2.25500E-01	0.0439	2.25500E-01	0.0439
nu(nu-1) (nu-4)/5!	3.09000E-02	0.0987	3.09000E-02	0.0987
nu(nu-1) (nu-5)/6!	2.10000E-03	0.2180	2.10000E-03	0.2180

spontaneous and induced fission multiplicity and moments. print table 117

	----- by number -----			----- by weight -----			error
	fissions	neutrons	multiplicity fraction	fissions	fission neutrons	multiplicity fraction	
nu = 0	700	0	6.90949E-02	3.25400E-02	0.00000E+00	6.90949E-02	0.0372
nu = 1	2301	2301	2.27125E-01	1.06964E-01	1.06964E-01	2.27125E-01	0.0197
nu = 2	3286	6572	3.24351E-01	1.52752E-01	3.05504E-01	3.24351E-01	0.0161
nu = 3	2558	7674	2.52492E-01	1.18910E-01	3.56731E-01	2.52492E-01	0.0186
nu = 4	1059	4236	1.04531E-01	4.92283E-02	1.96913E-01	1.04531E-01	0.0300
nu = 5	205	1025	2.02349E-02	9.52956E-03	4.76478E-02	2.02349E-02	0.0695
nu = 6	22	132	2.17155E-03	1.02269E-03	6.13611E-03	2.17155E-03	0.2131
total	10131	21940	1.00000E+00	4.70946E-01	1.01990E+00	1.00000E+00	0.0072

factorial moments	by number		by weight	
nu	2.16563E+00	0.0054	2.16563E+00	0.0054
nu(nu-1)/2!	1.94393E+00	0.0115	1.94393E+00	0.0115
nu(nu-1)(nu-2)/3!	9.16395E-01	0.0216	9.16395E-01	0.0216
nu(nu-1) (nu-3)/4!	2.38279E-01	0.0426	2.38279E-01	0.0426
nu(nu-1) (nu-4)/5!	3.32642E-02	0.0932	3.32642E-02	0.0932
nu(nu-1) (nu-5)/6!	2.17155E-03	0.2130	2.17155E-03	0.2130

In the above problem, there were 10000 source histories; all were spontaneous fissions. There were 21512 spontaneous fission neutrons produced. The number of source particles and the source weight listed in the problem summary table for neutrons is also 21512 and 2.1512E+00. Also, from the problem summary table for neutrons, there were 131 induced fissions, producing 428 fission neutrons.

In the second Print Table 117, there are 10000 + 131 = 10131 fissions. There are 21512 + 428 = 21940 fission neutrons. For nu = 0, the multiplicity fraction is 700 / 10131 = 0.0690949. The total multiplicity fraction always sums to 1. By-weight fissions sum to 10131 / 21512 = 0.470946. By-weight fission neutrons sum to 21940 / 21512 = 1.01990.

The by-weight multiplicity fractions are the same as the by-number multiplicity fractions because analog capture is used in this problem and the entire source is spontaneous fission.

If SDEF PAR = -SF is used, the tallies, summary information, and some entries in Print Table 117 are normalized by source history. By-weight fissions is 10131 / 10000 = 1.01310 instead of 0.470946. By-weight fission neutrons is 2.19400 instead of 1.01990. The by-weight multiplicity fractions are divided by the total fission weight, 10131.0, to sum to unity.

The first moment is nu = 21940 / 10131 = 2.16563. The second moment is $(2 \times 1 / 2! \times 3286 + 3 \times 2 / 2! \times 2558 + 4 \times 3 / 2! \times 1059 + 5 \times 4 / 2! \times 205 + 6 \times 5 / 2! \times 22) / 10131 = 1.94393$. The third moment is $(3 \times 2 \times 1 / 3! \times 2558 + 4 \times 3 \times 2 / 3! \times 1059 + 5 \times 4 \times 3 / 3! \times 205 + 6 \times 5 \times 4 /$

$3! \times 22) / 10131 = 0.916395$. The fourth moment is $(4 \times 3 \times 2 \times 1 / 4! \times 1059 + 5 \times 4 \times 3 \times 2 / 4! \times 205 + 6 \times 5 \times 4 \times 3 / 4! \times 22) / 10131 = 0.238279$. The fifth moment is $(5 \times 4 \times 3 \times 2 \times 1 / 5! \times 205 + 6 \times 5 \times 4 \times 3 \times 2 / 5! \times 22) / 10131 = 0.0332642$. The sixth moment is $6 \times 5 \times 4 \times 3 \times 2 \times 1 / 6! \times 22 / 10131 = 0.00217155$.

3.4. Multiple Particles on SDEF Card

Multiple-source-particle types may be specified in fixed-source problems. PAR on the SDEF card may be either a distribution or a dependent distribution.

3.4.1. Source Particle Type as the Independent Variable

```
sdef par=d1 pos fpar d2 erg fpar d3
si1 L h n
sp1 2 1
sb1 1 2
ds2 L 0 0 0 15 0 0
ds3 L 2 3
```

The particle types are protons (at 0,0,0, energy 2 MeV) and neutrons (at 15,0,0, energy 3 MeV).

3.4.2. Source Particle Type as a Dependent Variable

```
sdef par=fpos d2 pos=d1 erg fpos d3
si1 L 0 0 0 15 0 0
sp1 2 1
sb1 1 2
ds2 L h n
ds3 L 2 3
```

The source particles are protons and neutrons, depending on the problem source positions. This source tracks the source described in Section 3.4.1 exactly.

3.4.3. Additional Capabilities and Cautions

- The characters L, S, Q, F, and T are reserved as SI card options. L = discrete source variables, S = distribution numbers, etc. If the first entry on the SI card is L, S, Q, F, or T, it will be interpreted as a distribution option. To use source particle types L, S, Q, F, or T, either the corresponding particle numbers (10, 33, 30, 27, or 32) must be used or L, S, Q, F, or T must be used as the second or later particle type. Generally, it is best to specify the discrete source variable option; therefore, L will be the first entry, followed by the particle types. A second L will be interpreted correctly as particle type L. For example,

```
SI99 L -H N L Q F T S .
```

- Antiparticles may be designated. For example,

```
SI77 L -E N -H .
```

- Either characters (n, p, e, h, d, s, t, a, etc.) or numbers (1, 2, 3, 9, 31, 32, 33, 34, etc.) may be used. For example,

SI98 L -H 3 -32 N .

- Spontaneous fission may be used as a particle type. For example,

SI87 L SF N .

- Particle types may be listed multiple times to give them different energy distributions, angular distributions, etc., in different parts of the problem. For example,

SI23 L N n 1 n N .

3.4.4. Tally and Summary Table Normalizations

Tallies are normalized by dividing the total source weight by the number of source histories. Weight (WGT on the SDEF card) cannot be a source distribution (either independent or dependent). The weight of particles in the summary tables is controlled by the SI, SP, SB, and DS cards for the particle distribution. In the example shown in Section 3.4.1,

```
sdef par=d1 pos fpar d2 erg fpar d3
si1 L h n
sp1 2 1
sb1 1 2
ds2 L 0 0 0 15 0 0
ds3 L 2 3 .
```

The total source weight is $WGT = 1.0$ by default. From the SP1 card, the weight of the neutrons that are produced is 0.3333 and the weight of the protons that are produced is 0.6667. From the SB1 card, the total number of neutron tracks is $0.6667 \times NPS$ for neutrons and $0.3333 \times NPS$ for protons (where NPS is the number of source histories on the NPS card). The energy per source particle is normalized to the source particle weight for each source particle type. If the particle type is not a source particle (e.g., photons in the above problem), then the energy per source particle is normalized to the source particle weight of the lowest particle type. In this example, photon source energy would be normalized in the photon creation-and-loss summary table by 0.3333, which is the weight of the source neutrons produced.

Fission multiplicity and FT8 CAP capture tallies (Print Tables 117 and 118) “by number” quantities are always normalized by NPS, the number of histories run (NPS card). NPS generally equals the number of fissions, not fission neutrons, plus other source particles. The “by-weight” quantities are normalized by NPS for $PAR = SF$ and the “by-fission” neutrons (plus other source particles) for $PAR = -SF$.

Spontaneous fission has two normalizations: $PAR = SF$ and $PAR = -SF$. For $PAR = SF$, the normalization is total source weight, WGT, divided by the total neutron source weight: spontaneous fission neutrons plus other source neutrons.

3.5. Sources on Cylindrical Surfaces: SDEF

Cylindrical surface sources may be specified on the SDEF card. Furthermore, particle directions relative to the cylindrical source normal may be specified. The cylindrical surface can be, but

does not have to be, a cell-bounding problem surface. Likewise, a spherical surface source no longer has to be on a cell-bounding problem surface.

In MCNP and earlier MCNPX versions, the only way to specify a cylindrical surface source was to have a degenerate cylindrical volume source (radius = constant) that is not also a problem surface. Particle direction had to be isotropic from the source point.

3.5.1. Examples

The following examples now work, whereas all failed in previous MCNP and MCNPX versions.

Cylindrical problem surface with default cosine distribution relative to surface normal:

```
SDEF pos = 0 0 0   rad = 1   ext = d1   axs = 1 0 0   sur = 5 .
```

Cylindrical problem surface with specified angle distribution relative to surface normal:

```
SDEF pos = 0 0 0   rad = 1   ext = d1   axs = 1 0 0   sur = 5   dir = d2 .
```

Cylindrical surface (degenerate volume source) with specified angle distribution relative to surface normal:

```
SDEF pos = 0 0 0   rad = 1   ext = d1   axs = 1 0 0   dir = d2 .
```

Spherical surface (degenerate volume source) with specified angle distribution relative to surface normal:

```
SDEF pos = 0 0 0   rad = 1   dir = d2 .
```

3.5.2. Additional Information and Cautions

If the cylindrical surface is a problem surface, then the surface number must be specified on the SDEF card with the SUR parameter.

If both DIR and VEC are specified, then particle directions are relative to VEC rather than to the cylindrical surface normal.

All former capabilities remain the same:

- volume sources have a default isotropic direction;
- particle directions are relative to VEC if VEC is specified;
- only capabilities that formerly were disallowed are different:
 - SUR may be specified on a cylindrical surface, and the default VEC is the surface normal;
 - DIR may be specified without VEC (so that VEC defaults to the surface normal) for spheres and cylinders; and

- the outward normal to cylindrical surfaces is generated whenever DIR is specified and VEC is not.

3.6. Repeated Structures Source Specifications: SI

The CEL source specification for repeated structures geometries now is consistent with the tally specification. The old MCNP4C specification still works, but the MCNPX is

```
SDEF CEL=d3 POS=0 6 0 EXT=d1 RAD=d2 AXS= 0 1 0
SI3 L (1<10[0 0 0]<11) (1<10[1 0 0]<11) (1<10[2 0 0]<11)
      (1<10[0 1 0]<11) (1<10[1 1 0]<11) (1<10[2 1 0]<11) .
```

3.7. Translated Sources with Dependence

MCNPX allows translating sources to different locations with the TR option on the SDEF card. This capability is most useful for setting up the source as an accelerator beam and then using the translation as a distribution to repeat the accelerator source at different locations and orientations. The TR option on the SDEF card can be dependent on other source variables. For example, the particle type can depend on the translated source location:

```
SDEF      CEL=FTR=D3      PAR=FTR=D1      TR=D2 .
```

Or the translated source location can be a dependent distribution function of cell:

```
SDEF      CEL=D2      TR=FCEL=D5 .
```

Thus, the TR parameter on the SDEF card is consistent with the other source parameters.

4.0. TALLY FEATURES

The MCNPX tally extensions provide a wide range of significant capabilities. Note that logarithmic interpolation (Section 5.1) is particularly useful for many tally cards. The applicable tally input cards are found in parentheses after the features they control.

- PHTs with variance reduction (F8);
- Default dose functions (DF);
- Lattice tally speedup by orders of magnitude (F);
- Radiography tallies: translate new MCNP5 FIP, FIR, and FIC radiography input cards as MCNPX radiography tallies PI, TIR, and TIC;
- Proton and photonuclear reaction multipliers (FM);
- Cosine bins that may be specified in degrees and for F2 tallies (C);
- Pulse-height light tally with anticoincidence: FT8 PHL;
- Coincidence capture tally: FT8 CAP;
- Residual nuclei tally: FT8 RES.

4.1. Pulse-Height Tallies with Variance Reduction

MCNPX allows variance reduction techniques (VRTs) with F8 PHTs. Unlike standard Monte Carlo tallies, which score events as they occur, PHTs combine the energy deposition of many events in a single Monte Carlo “history.” The entire history tree must score, not just a single event in the tree. Further, VRT events such as Russian roulette can kill the entire tree if they occur after a physical event such as photon pair production.

MCNPX enables VRTs with PHTs. * Results are very problem dependent, and variance reduction is more challenging than with other MCNPX tallies. On a space satellite problem, calculations were sped up by two orders of magnitude.† Although the MCNPX capability greatly enhances most F8 PHT calculations, it has not been extended to all VRTs or physics combinations. See Section 4.1.1, “Future Work.”

No user interface changes are required to use VRTs with PHTs. If VRTs are used with PHTs, a fatal error no longer occurs unless the VRTs are incompatible with PHTs. Several warning messages occur if it appears that the VRTs will be inefficient with PHTs. If no VRTs are specified, MCNPX uses the MCNP4C3 analog algorithm without constructing PHT trees.

4.1.1. Future Work

PHTs work with VRTs in the most widely used F8 PHT applications: electrons and photons. They do not work with other particle types and have other extensions that must await further funding. Among these future work items are

- enable neutrons and other particles to use VRTs with PHTs;
- enable more than a single F8 tally per problem;
- enable DXTRAN and SPABI VRTs; and
- extend to FT special treatments, particularly the light tally with anticoincidence, residual nuclei, and capture options (FT PHL, RES, and CAP options).

4.2. Default Dose Functions (DF)

The DE/DF dose function cards are unchanged but now have extensions. As before, dose conversions may be input as a table. Note that the interpolation $\text{int} = \text{log}$ or $\text{int} = \text{lin}$ may be placed anywhere, and $n = \text{tally number}$, which implies particle type.

```
DEn E1 E2 int E3 ...
DFn F1 int F2 F3 ...
```

The dose conversion capability is extended to provide standard default dose functions. These are invoked by omitting the DE card and using keywords on the DF card

* John S. Hendricks and Gregg W. McKinney, “Pulse-Height Tallies with Variance Reduction,” Los Alamos National Laboratory report LA-UR-04-8431 (2004).

† John S. Hendricks and Jane M. Burward-Hoy, “Monte Carlo Radiation Detector Modeling in Space Systems,” Los Alamos National Laboratory report LA-UR-05-0278 (2005).

DFn iu=j fac=F int ic=I ,

where all of the following entries are optional.

iu = 1 = US units (rem/h)

iu = 2 = international units (sieverts/h)

Default: iu = 2 international units (sieverts/h)

fac = normalization factor for dose (acr is also accepted instead of fac).

fac = -1 = normalize results to $Q = 20$ by dividing the parametric form of Q [$5.0+17.0 \times \exp(-(\ln(2E)) \times 2/6)$] from ICRP60 (1990), paragraph A12.

fac = -2 = apply LANSCE albatross response function.

Default: fac = 1.0.

int = "log" or "lin" results in "log" or "lin" interpolation of energy; the dose function is always linear. That is, "lin" results in "linlin" interpolation, and "log" results in "loglin" interpolation.

Default: for ic = 10, 40: log

for ic = 20,31-39: recommended analytic parameterization.

ic = i = standard dose function.

i neutron dose function

10 = ICRP-21 1971

20 = NCRP-38 1971, ANSI/ANS-6.1.1-1977

31 = ANSI/ANS-6.1.1-1991 (AP anterior-posterior)

32 = (PA posterior-anterior)

33 = (LAT side exposure)

34 = (ROT normal to length and rotationally symmetric)

40 = ICRP-74 1996 ambient dose equivalent

i photon dose function

10 = ICRP-21 1971

20 = Claiborne & Trubey, ANSI/ANS 6.1.1-1977

31 = ANSI/ANS-6.1.1-1991 [AP (anterior-posterior)]

32 = PA (posterior-anterior)

33 = (LAT side exposure)

34 = (ROT normal to length and rotationally symmetric)

35 = (ISO isotropic)

Default: ic = 10

Examples:

DF4

DF0 ic 40 iu 1 lin fac 123.4

DF1 iu=2 acr=-2 log ic=34

4.3. Lattice Tally Speedup (F)

With no change in the user interface, input files with large lattice tallies run 10 to 1000 times faster than in MCNP4C3 if the following apply:

- The lattice is specified fully on the cell fill card, e.g., FILL -50:50 -50:50 -50:50.
- The tally chain refers to no more than one cell at each level, except for the lattice cell, which must include the entire range of all indices specified on the corresponding FILL card:

F4:p (1 < 2 < 3[-50:50 -50:50 -50:50] < 4) .

The following,

F4:p (1 < 2 < 3[-50:50 -50:50 -50:50] < 4 5) ,

will not work because two cells, 4 and 5, were specified at the top level.

Example:

The following example of a simple input file runs 70 times faster with MCNPX than with MCNPX 2.4.0 and MCNP4C versions.

```
21x21x21 void lattice of balls
11 0 -31 u=1 imp:p=1
12 0 31 u=1 imp:p=1
16 0 -32 u=2 imp:p=1
    lat=1 fill= -10:10 -10:10 -10:10 1 9260R
17 0 -33 fill=2 imp:p=1
18 0 33          imp:p=0

31 sph 0 0 0 .5
32 rpp -1 1 -1 1 -1 1
33 rpp -21 21 -21 21 -21 21

mode      p
print
prdmp 2j -3
sdef
nps      10000
f4:p (11<16[-10:10 -10:10 -10:10]<17)
```

Larger lattices and nested lattices offer even more dramatic speedups but take longer to demonstrate than the simple example shown.

4.4. Radiography Tally (FIP, FIR, FIC)

Radiography tallies may be input with either the standard MCNPX card names (PI, TIR, TIC) or the MCNP5 card names (**FIP, FIR, and FIC**). In all cases, the radiographical plane is specified with C and FS cards for the s and t axes. The tally number is n and the particle type is p, which may be either neutron, N, or photon, P.

4.4.1. Pinhole Radiography

FIPn:p *X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3*

PIIn:p *X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3* ,

where

X1 Y1 Z1 = coordinates of the pinhole,
R0 = 0,
X2 Y2 Z2 = reference coordinates (center of object),
F1 = collimator radius,
F2 = pinhole size, and
F3 = distance from pinhole to detector grid defined by C and FS cards.

4.4.2. Transmitted Image Projection

Rectangular grid:

FIRn:p *X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3*

TIRn:p *X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3*

Cylindrical grid:

FICn:p *X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3*

TICn:p *X1 Y1 Z1 R0 X2 Y2 Z2 F1 F2 F3* ,

where

X1 Y1 Z1 = coordinates of center of grid defined by C and FS cards,
R0 = 0,
X2 Y2 Z2 = reference coordinates (center of object),
F1 = -1 / 0 = scattered only/direct + scattered—contributions to detector,
F2 = radial field of view, and
F3 = 0 / -1 contributions scored at center/random—on grid.

4.5. Photonuclear and Proton Reaction Multipliers (FM)

Photonuclear and proton cross sections may be used in tally multipliers on the FM card. For example,

M102 92235 1 pnlb = 27u

F2:P 1
 FM2 (-1 102 18 1018) .

Photonuclear cross-section reaction numbers all are positive, unlike the photoatomic reaction numbers, which are negative. The principal photonuclear cross sections are the following: 1 = total, 2 = nonelastic, 3 = elastic, 4 = heating, and >4 = various reactions such as 18 = (γf). The photonuclear yields (multiplicities) for various secondary particles are specified by adding 1000 times the secondary particle number to the reaction number. For example, 31001 is the total yield of deuterons (particle type d = 31), 34001 is the total yield of alphas (particle type α = 34), and 1018 is the total number of neutrons (particle type n = 1) from fission.

Proton reaction numbers are similar to the neutron reaction numbers—all positive. The principal proton cross sections are ± 1 = total, ± 2 = nonelastic, ± 3 = elastic, ± 4 = heating, >4 = various reactions. On the LA150H proton library, the only available reaction is mt = 5 and its multiplicities, 1005, 9005, 31005, etc. The multiplicity reaction numbers are specified by adding 1000 times the secondary particle number to the reaction number. For interaction reaction mt = 5, the multiplicities are 1005 for neutrons, 9005 for protons, 31005 for deuterons, etc. The proton multiplicity, mt = 9001, 9004, 9005, etc., is generally available, along with the total cross-section and heating number, mt = 1, mt = 4.

It is always wise to plot the desired cross sections first to see if they are available with the expected reaction numbers in the data library. The tally multipliers treat the data the same as the data are treated in transport: the cross section at the lowest energy is extended down to $E = 0$ for protons with mt < 0; the cross section at the highest energy of the table is extended to $E = \infty$ for proton interaction cross sections with mt < 0, and for photonuclear interaction cross sections, mt < 1000. These extrapolations can be seen in the cross-section plots.

4.6. Expanded Cosine Specification (C)

Cosines may be specified in degrees. They also may be specified with surface flux (F2) tallies as

*C2 150 120 90 60 30 0 .

The * on the C2 card interprets cosines as in degrees. Entries must be such that the cosine is monotonically increasing.

4.7. Pulse-Height Light Tally with Anticoincidence: FT8 PHL

Pulse-height (F8) tallies may be based on energy/light deposition in one or two other regions as specified via one or two F6 tallies. Thus, this tally is dependent on results from another tally, which works because the F8 tally is posted at the end of the particle history where the F6 tallies are accumulated along each track of the particle history. The format of the FT PHL card is

FT8 PHL N T_{A1} B_{A1} T_{A2} B_{A2} ... M T_{B1} B_{B1} T_{B2} B_{B2} ... ,

where

- N = number of F6 tallies for the first detector region,
- $T_{A1} B_{A1} \dots$ = pairings of tally number and f-bin number for the N F6 tallies of the first detector region,
- M = number of F6 tallies for the second detector region, and
- $T_{B1} B_{B1} \dots$ = pairings of tally number and f-bin number for the M F6 tally of the second detector region.

When M is nonzero, indicating the use of two detector regions, an FU card is required for the F8 tally. The entries on the FU card are presented in units of electron-equivalent light (MeV_{ee}) and must increase monotonically. The particle type indicated on the F8 tally does not matter because this tally allows a combination of light output from various particle types. If B_{An} is zero, then the number of cell bins on the F8 card must match that on the corresponding T_{An} tally card. Setting B_{An} to zero allows for a lattice pulse-height PHL tally.

Examples:

Case 1

```
F8:n 5
FT8  PHL 1 6 1 0
E8   1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0
F6:e 5
DE6  LIN 1.0 1.5 2.0 2.5 3.0 3.5 10.0
DF6  LIN 1.0 1.1 1.2 1.3 1.4 1.5 1.6
FT6  GEB A B C
```

Case 2

```
F8:n 5
FT8  PHL 1 6 1 1 16 1
E8   1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0
FU8  1.5 2.5 3.5 4.5 5.5 6.5 7.5 8.5
F6:e 5
DE6  LIN 1.0 1.5 2.0 2.5 3.0 3.5 10.0
DF6  LIN 1.0 1.1 1.2 1.3 1.4 1.5 1.6
FT6  GEB A B C
F16:e 6
DE16 LIN 1.0 1.5 2.0 2.5 3.0 3.5 10.0
DF16 LIN 1.0 1.1 1.2 1.3 1.4 1.5 1.6
FT16 GEB A B C
```

In both cases, the F6 tallies convert energy deposition to equivalent light (units in millielectron volts). SD cards are not required with the F6 tallies because these divisors renormalize only the printed output for the F6 tallies and not the values stored in the tally arrays (thus, the F8 tally will result in the same value, regardless of whether the F6 tally has an SD card). The DE/DF conversion is based on the incident particle energy, and the values on the DF card should be the dL/dE for that incident particle energy. Thus, the F6 tally will multiply the dL/dE values by the energy deposition to give the light output (ΔL) summed over each track. Also, no energy bins exist for the F6 tallies. The F8 tally uses the total light output. Energy bins (E6 card) can be

added, but the F8 tally will use the value from the total bin. Similarly, for other bins associated with the F6 tally, in each case, the TFC bin is used to extract the value for the F8 tally (see the TF card to alter this). The FT GEB cards are used to perform Gaussian broadening on these tally values; however, this process is done only at the end of the particle history to determine the light output value used in the PHT.

In Case 1, the electron light output from only one region (cell 5) is used to subdivide the PHT. In this case, a pulse of 1 (input source weight) is put into the first E8 bin when the light output in cell 5 is <1 MeV. It is placed in the second E8 bin when the light output is between 1 and 2 MeV, etc. A zero F6 tally will result in no F8 tally.

In Case 2, the light output from two regions (cells 5 and 6) is used to subdivide the PHT. This case is useful for coincidence/anticoincidence applications. A pulse of 1 (input source weight) is put into the first E8 bin and into the first FU8 bin when the light output in cell 5 is <1.0 MeV *and* the light output in cell 6 is <1.5 MeV. This pulse is put into the first E8 bin and into the second FU8 bin when the light output in cell 5 is <1.0 MeV *and* the light output in cell 6 is between 1.5 and 2.5 MeV. A zero light output in both cells will result in no F8 tally. A zero light output in cell 5 (tally 6) with a nonzero light output in cell 6 (tally 16) will result in a pulse in the corresponding FU8 bin. Similarly, for a zero light output in cell 6 and a nonzero light output in cell 5, a pulse will be put into the corresponding E8 bin. The E8 and FU8 bins do not have to be the same and typically would not be unless the detector regions were of similar material and size. Separate F6 tallies (as in Case 2, F6 and F16) are needed only when the two regions have different light conversion functions. If the two regions are of the same material, then a single F6 tally can be used as follows.

```

F8:n 5
FT8  PHL 1 6 1 1 6 2
E8    1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0
FU8   1.5 2.5 3.5 4.5 5.5 6.5 7.5 8.5
F6:e  5 6
DE6   LIN 1.0 1.5 2.0 2.5 3.0 3.5 10.0
DF6   LIN 1.0 1.1 1.2 1.3 1.4 1.5 1.6
    
```

Currently, it is not important to determine what cell is listed on the F8 card because this tally is made only at the end of a particle history and depends only on the tally results of the listed F6 tallies. Having multiple cells listed on the F8 card is meaningful only when the f-bin parameter (i.e., B_{An} or B_{Bn}) of the FT PHL option is zero, indicating a lattice grid of detector regions. Otherwise, each additional F8 cell bin simply will be a duplicate of the first cell bin.

4.8. Coincidence Capture Tally (FT8 CAP)

The FT8 capture tally scores the number of captures in specified combinations of nuclides at the end of each history. The tally is particularly useful for neutron coincidence detectors. In addition, captures may be written to an auxiliary output file, PTRAC. Section 5.5 describes the PTRAC capture file:

```
FT8 [-Mc] [-Mo] I1 I2 ... [Gate td tw] ,
```

where

Mc = optional maximum number of captures (default = 21),
 Mo = optional maximum number of moments (default = 12),
 In = capture nuclide(s) such as 3006 or 5010 for ${}^6\text{Li}$ or ${}^{10}\text{B}$, and
 Gate td tw = optional time gate with pre-delay time, td, and time gate width, tw.

Example:

```
F8:n  2 (5 6) 7 T
FT8   cap  3006 5010
T8    1 7LOG 1E8 .
```

In this example, captures and moments are tallied in cells 2, 7, in the combination of 5 and 6 and in the total over cells 2, 5, 6, 7. The captures by either ${}^6\text{Li}$ or ${}^{10}\text{B}$ are tallied. Results are tabulated in time bins at 1, 10, 100, 1000, 1e4, 1e5, 1e6, 1e7, and 1e8 shakes—that is, in the range of 10 ns to 1 s.

4.8.1. Restrictions

Coincidence counting of capture multiplicities and moments requires analog capture: CUT:N 2J 0 0. Calculations must be totally analog, with no variance reduction. Fission multiplicity also is required: PHYS:N J 100 3J -1. An FT8 CAP tally in an input file automatically will set analog capture, fission multiplicity, and exit with error messages if variance reduction is used. The capture multiplicities and moments are stored in 80 cosine bins, which are printed out with the F8 tally. A much more readable table of capture multiplicities and moments is given in Print Table 118. The captures and moments can be compared with Print Table 117, which has the spontaneous-fission source and induced-fission summaries of fission neutrons and moments (Section 3.3.3).

The capture tallies may be written to a PTRAC file for further analysis by auxiliary codes. See Section 5.5 on the PTRAC card extensions.

4.8.2. Interpreting Capture Tally Output

The FT8 CAP coincidence capture tally option produces both a standard tally, which is generally unreadable, and a coincidence capture table, Print Table 118. An example is provided to help in the interpretation of this table.

neutron captures, moments & multiplicity distributions. tally 8 print table
118

cell: 999

neutron captures on 3he

	histories	captures by number	captures by weight	multiplicity by number	fractions by weight	error
captures = 0	700	0	0.00000E+00	7.00000E-02	3.25400E-02	0.0364
captures = 1	2285	2285	1.06220E-01	2.28500E-01	1.06220E-01	0.0184
captures = 2	3223	6446	2.99647E-01	3.22300E-01	1.49823E-01	0.0145
captures = 3	2489	7467	3.47109E-01	2.48900E-01	1.15703E-01	0.0174
captures = 4	1022	4088	1.90033E-01	1.02200E-01	4.75084E-02	0.0296
captures = 5	209	1045	4.85775E-02	2.09000E-02	9.71551E-03	0.0684
captures = 6	51	306	1.42246E-02	5.10000E-03	2.37077E-03	0.1397
captures = 7	12	84	3.90480E-03	1.20000E-03	5.57828E-04	0.2885
captures > 7	9	73	3.39345E-03	9.00000E-04	4.18371E-04	0.3332
total	10000	21794	1.01311E+00	1.00000E+00	4.64857E-01	0.0056

factorial moments

by number

by weight

3he	2.17940E+00	0.0056	1.01311E+00	0.0056
3he(3he-1)/2!	2.01890E+00	0.0128	9.38499E-01	0.0128
3he(3he-1)(3he-2)/3!	1.06390E+00	0.0291	4.94561E-01	0.0291
3he(3he-1)....(3he-3)/4!	3.93800E-01	0.0744	1.83061E-01	0.0744
3he(3he-1)....(3he-4)/5!	1.34100E-01	0.1636	6.23373E-02	0.1636
3he(3he-1)....(3he-5)/6!	4.43000E-02	0.2666	2.05932E-02	0.2666
3he(3he-1)....(3he-6)/7!	1.12000E-02	0.3808	5.20640E-03	0.3808
3he(3he-1)....(3he-7)/8!	1.70000E-03	0.5548	7.90257E-04	0.5548

The capture tally input for this problem was

```
F8:n 999          input F8 card
FT8  CAP -8 -8 2003 input FT8 CAP card
```

Note that the line captures > 7 9 73 indicate that nine histories had eight or more neutrons captured. This implies that 8 histories had $8 \times 8 = 64$ neutrons captured and 1 history had 1×9 neutrons captured, for a total of 73 neutrons captured. The table of captures evidently was too short, and the problem should have been run with FT8 CAP -9 -9 or even more captures and moments. Not specifying enough capture rows affects only the captures > 7 lines and the error estimate on the totals capture line; all other information is correct as if more captures and moments were listed.

As an interpretation of the neutron captures on the 3he table, Column 1 is the number of histories according to the number of captures by the designated material (2003 = 3he) in the designated cell (999). This number sums to the total number of source histories for the problem, nps = 10000.

Column 2 is the number of captures by 2003 in cell 999 = 21794. Because analog capture is the default for F8 tallies, the total weight captured is also 21794.

Column 3 is the total weight captured divided by the tally normalization. For SDEF PAR = -SF, the tally normalization is the number of source histories = number of spontaneous fissions = 10000. For SDEF PAR = -SF, column 3 would be $21794.0 / 10000 = 2.17940$. In this problem, SDEF PAR = SF, and the tally normalization is the source particles = spontaneous fission neutrons = 21512. Thus, captures by weight are $21794.0 / 21512 = 1.01311$.

Column 4 is the multiplicity fraction by number, which is Column 1 divided by the number of source histories. The total is always 1.00000.

Column 5 is the multiplicity fraction by weight, which is the weight of histories undergoing capture divided by the tally normalization. For SDEF PAR = -SF, this fraction would be $10000.0 / 10000 = 1.00000$. In this problem, SDEF PAR = SF and the multiplicity fraction by weight is $10000.0 / 21512 = 0.464857$.

The interpretation of the factorial moments table now follows.

The first moment by number is the number of captures divided by the number of source histories = $21794 / 10000 = 2.17940$.

The first moment by weight is the total weight of capture divided by the tally normalization. For SDEF PAR = -SF, this moment would be $21794.0 / 10000 = 21794.0$. In this problem, SDEF PAR = SF and the first moment by weight is $21794.0 / 21512 = 1.01311$.

The second moment is $N \times (N-1)/2$, where N is the number of captures. In this problem,

N	$N \times (N-1)/2$	histories	product
1	0	× 2285	= 0
2	1	× 3223	= 3223
3	3	× 2489	= 7467
4	6	× 1022	= 6132
5	10	× 209	= 2090
6	15	× 51	= 765
7	21	× 12	= 252
8	28	× 8	= 224
9	36	× 1	= 36
	sum		= 20189 ,

and the second moment by number is divided by the number of histories,

$$20189 / 10000 = 2.01890 \text{ .}$$

Because of analog capture, the second moment weight is 20189.0. The second moment by weight is divided by the tally normalization. For SDEF PAR = -SF, this moment would be $20189.0 / 10000 = 2.01890$, which is the same as the second moment by number. In this problem, SDEF PAR = SF, and the second moment by weight is

$$20189.0 / 21512 = 0.938499 \text{ .}$$

The seventh moment is

$$\begin{array}{rclclcl}
 7 \times 6 \times 5 \times 4 \times 3 \times 2 \times 1/7! & = & 1 & \times & 12 & = & 12 \\
 8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2/7! & = & 8 & \times & 8 & = & 64 \\
 9 \times 8 \times 7 \times 6 \times 5 \times 4 \times 3/7! & = & 36 & \times & 1 & = & 36 \\
 \text{sum} & & & & = & & 112 ;
 \end{array}$$

thus, $112 / 10000 = 0.0112$.

The eighth moment is

$$\begin{array}{rclclcl}
 8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2 \times 1/8! & = & 1 & \times & 8 & = & 8 \\
 9 \times 8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2/8! & = & 9 & \times & 1 & = & 9 \\
 \text{sum} & & & & = & & 17 ;
 \end{array}$$

thus, $17 / 10000 = 0.0017$.

And the ninth moment is

$$9 \times 8 \times 7 \times 6 \times 5 \times 4 \times 3 \times 2 \times 1/9! = 1 \times 1 = 1 ;$$

thus, $1 / 10000 = 0.0001$.

4.8.3. FT8 Capture Tallies with Time Gating

The coincidence capture tally optionally allows specification of predelay and gate width* with the “gate” keyword on the FT8 card. The “gate” keyword may appear anywhere after the “cap” keyword and is part of the “cap” command. Immediately following, the “gate” keyword must be the predelay time and the total gate width, both in units of shakes (1.0e-8 s).

The addition of the predelay and time gate width changes the capture tally scoring. When a neutron is captured at time $t0$ in the specified cell by the specified nuclide (22 and $^3\text{He} = 2003$ in all three tallies below), the gate is “turned on.” If the predelay is $t1$ and the gate width is $t2$, then all captures between $t0 + t1$ and $t0 + t1 + t2$ are counted. For a history with no captures, no events are scored. With one capture, 0 events are scored. With two captures, the first turns on the time gate are at time $t0$ and scores 0; the second will score one event if it is captured between $t0 + t1$ and $t0 + t1 + t2$ or score another 0 if outside the gate.

Other entries after the “cap” keyword may be placed in any order, as shown in the following examples. The negative entries change the allowed number of captures and moments (defaults 21 and 12 are changed to 40 and 40 in F78 below). The list of capture nuclides ($^3\text{He} = 2003$ in all three tallies below) also may be placed anywhere after “cap.”

* Martyn T. Swinhoe, John S. Hendricks, and Douglas R. Mayo, “MCNPX for Neutron Multiplicity Detector Simulation,” Los Alamos National Laboratory report LA-UR-04-8025 (2004).

Examples for three capture tallies now follow. The capture tally without gating (f18) is shown for reference. An infinite gate (F38) results in a very different Print Table 118: the number of captures is the same, but the moments are offset by one. A finite gate (F78) has fewer captures, as expected.

Example 1: Capture Tally without Gate

Input:

```
f18:n 22
ft18 cap 2003
```

Output:

```
1 neutron captures, moments and multiplicity distributions. tally 18
print table 118
```

```
weight normalization by source histories = 20000
```

```
cell: 22
```

```
neutron captures on 3he
```

	histories	captures by number	captures by weight	multiplicity by number	fractions by weight	error
captures = 0	13448	0	0.00000E+00	6.72400E-01	6.72400E-01	0.0049
captures = 1	5550	5550	2.77500E-01	2.77500E-01	2.77500E-01	0.0114
captures = 2	588	1176	5.88000E-02	2.94000E-02	2.94000E-02	0.0406
captures = 3	238	714	3.57000E-02	1.19000E-02	1.19000E-02	0.0644
captures = 4	94	376	1.88000E-02	4.70000E-03	4.70000E-03	0.1029
captures = 5	40	200	1.00000E-02	2.00000E-03	2.00000E-03	0.1580
captures = 6	26	156	7.80000E-03	1.30000E-03	1.30000E-03	0.1960
captures = 7	8	56	2.80000E-03	4.00000E-04	4.00000E-04	0.3535
captures = 8	5	40	2.00000E-03	2.50000E-04	2.50000E-04	0.4472
captures = 9	1	9	4.50000E-04	5.00000E-05	5.00000E-05	1.0000
captures = 12	1	12	6.00000E-04	5.00000E-05	5.00000E-05	1.0000
captures = 16	1	16	8.00000E-04	5.00000E-05	5.00000E-05	1.0000
total	20000	8305	4.15250E-01	1.00000E+00	1.00000E+00	0.0128

```
factorial moments
```

```
by number
```

```
by weight
```

3he	4.15250E-01	0.0128	4.15250E-01	0.0128
3he(3he-1)/2!	1.59300E-01	0.0651	1.59300E-01	0.0651
3he(3he-1)(3he-2)/3!	1.47900E-01	0.2165	1.47900E-01	0.2165
3he(3he-1) ... (3he-3)/4!	1.87750E-01	0.5063	1.87750E-01	0.5063
3he(3he-1) ... (3he-4)/5!	2.96500E-01	0.7493	2.96500E-01	0.7493
3he(3he-1) ... (3he-5)/6!	4.61900E-01	0.8727	4.61900E-01	0.8727
3he(3he-1) ... (3he-6)/7!	6.15800E-01	0.9311	6.15800E-01	0.9311
3he(3he-1) ... (3he-7)/8!	6.68950E-01	0.9626	6.68950E-01	0.9626
3he(3he-1) ... (3he-8)/9!	5.83050E-01	0.9812	5.83050E-01	0.9812
3he(3he-1) ... (3he-9)/10!	4.03700E-01	0.9918	4.03700E-01	0.9918
3he(3he-1) ... (3he-10)/11!	2.19000E-01	0.9972	2.19000E-01	0.9972
3he(3he-1) ... (3he-11)/12!	9.10500E-02	0.9994	9.10500E-02	0.9994

Example 2: Infinite Gate

Input:

```
f38:n 22
ft38 cap 2003 gate 0 le11
```

Output:

1 neutron captures, moments and multiplicity distributions. tally 38
 print table 118

weight normalization by source histories = 20000

cell: 22

neutron captures on 3he

time gate: predelay = 0.0000E+00 gate width = 1.0000E+11

	pulses in gate	occurrences histogram	occurrences by number	occurrences by weight	pulse fraction by number	pulse fraction by weight	error
captures = 0	0	6552	0	0.00000E+00	3.27600E-01	3.27600E-01	0.0101
captures = 1	1	1002	1002	5.01000E-02	5.01000E-02	5.01000E-02	0.0308
captures = 2	2	414	828	4.14000E-02	2.07000E-02	2.07000E-02	0.0486
captures = 3	3	176	528	2.64000E-02	8.80000E-03	8.80000E-03	0.0750
captures = 4	4	82	328	1.64000E-02	4.10000E-03	4.10000E-03	0.1102
captures = 5	5	42	210	1.05000E-02	2.10000E-03	2.10000E-03	0.1541
captures = 6	6	16	96	4.80000E-03	8.00000E-04	8.00000E-04	0.2499
captures = 7	7	8	56	2.80000E-03	4.00000E-04	4.00000E-04	0.3535
captures = 8	8	3	24	1.20000E-03	1.50000E-04	1.50000E-04	0.5773
captures = 9	9	2	18	9.00000E-04	1.00000E-04	1.00000E-04	0.7071
captures = 10	10	2	20	1.00000E-03	1.00000E-04	1.00000E-04	0.7071
captures = 11	11	2	22	1.10000E-03	1.00000E-04	1.00000E-04	0.7071
captures = 12	12	1	12	6.00000E-04	5.00000E-05	5.00000E-05	1.0000
captures = 13	13	1	13	6.50000E-04	5.00000E-05	5.00000E-05	1.0000
captures = 14	14	1	14	7.00000E-04	5.00000E-05	5.00000E-05	1.0000
captures = 15	15	1	15	7.50000E-04	5.00000E-05	5.00000E-05	1.0000
total		8305	3186	1.59300E-01	4.15250E-01	4.15250E-01	0.0291

factorial moments	by number		by weight	
n	1.59300E-01	0.0651	1.59300E-01	0.0648
n(n-1)/2!	1.47900E-01	0.2165	1.47900E-01	0.2165
n(n-1)(n-2)/3!	1.87750E-01	0.5063	1.87750E-01	0.5062
n(n-1)(n-2) ... (n-3)/4!	2.96500E-01	0.7493	2.96500E-01	0.7492
n(n-1)(n-2) ... (n-4)/5!	4.61900E-01	0.8727	4.61900E-01	0.8726
n(n-1)(n-2) ... (n-5)/6!	6.15800E-01	0.9311	6.15800E-01	0.9311
n(n-1)(n-2) ... (n-6)/7!	6.68950E-01	0.9626	6.68950E-01	0.9626
n(n-1)(n-2) ... (n-7)/8!	5.83050E-01	0.9812	5.83050E-01	0.9812
n(n-1)(n-2) ... (n-8)/9!	4.03700E-01	0.9918	4.03700E-01	0.9918
n(n-1)(n-2) ... (n-9)/10!	2.19000E-01	0.9972	2.19000E-01	0.9972
n(n-1)(n-2) ... (n-10)/11!	9.10500E-02	0.9994	9.10500E-02	0.9994
n(n-1)(n-2) ... (n-11)/12!	2.80000E-02	1.0000	2.80000E-02	1.0000

Example 3: Finite Gate

Input:

```
f78:n 22
ft78 cap gate .5 .4 -40 -40 2003
```

Output:

```
1 neutron captures, moments and multiplicity distributions. tally 78
print table 118

weight normalization by source histories = 20000

cell: 22

neutron captures on 3he

time gate: predelay = 5.0000E-01 gate width = 4.0000E-01

      pulses      occurrences  occurrences      pulse fraction
      in gate histogram by number  by weight  by number  by weight  error
captures = 0  7837    0  0.00000E+00  3.91850E-01  3.91850E-01  0.0118
captures = 1   394   394  1.97000E-02  1.97000E-02  1.97000E-02  0.0666
captures = 2    67   134  6.70000E-03  3.35000E-03  3.35000E-03  0.1542
captures = 3     6    18  9.00000E-04  3.00000E-04  3.00000E-04  0.4082
captures = 4     1     4  2.00000E-04  5.00000E-05  5.00000E-05  1.0000

total          8305   550  2.75000E-02  4.15250E-01  4.15250E-01  0.0624

      factorial moments      by number      by weight
      n
      n(n-1)/2!  2.75000E-02  0.0716  2.75000E-02  0.0716
      n(n-1)(n-2)/3!  4.55000E-03  0.1654  4.55000E-03  0.1654
      n(n-1)(n-2) ... (n-3)/4!  5.00000E-04  0.4690  5.00000E-04  0.4690
      n(n-1)(n-2) ... (n-3)/4!  5.00000E-05  1.0000  5.00000E-05  1.0000
```

Scratch space is needed to save capture times during the course of a history. The times are stored temporarily in the capture and moment bins of the tally. If sufficient bins are unavailable, then the number of allowed captures and moments must be increased using the negative entries after the “cap” keyword. The message “ *** warning *** dimension overflow. Some pulses not counted.” is put in Print Table 118 if the space needs to be increased.

4.8.4. Possible Future Extensions of FT8 CAP Option

The coincidence counter capture tally model lacks many standard tally features to make the algorithm faster. Adding the following tally capabilities would be a straightforward extension:

- extension to particle types other than neutrons,
- tally cell and surface flagging,
- extension to other special tally treatment options on the FT card,
- tally segmenting,
- tally multipliers, and
- energy bins.

4.9. Residual Nuclei Tally: FT8 RES

Residual nuclei from nuclear interactions in the model physics energy range may be tallied with the FT tally special treatments RES option in conjunction with PHTs. The form of the FT card is

FT8 RES ,

or

FT8 RES Z₁ Z₂ .

The interaction of high-energy particles with target nuclei causes the production of many residual nuclei. The generated residual nuclei can be recorded to an F8 tally if used with an FT8 RES special-treatment option. The residuals are recorded at each interaction in the model physics; residual nuclei are not tabulated at collisions using table physics.

By default, the FT8 RES card will cause the corresponding F8 tally to have 2000+ user bins for each possible residual nucleus ZAID. The range of ZAID bins may be reduced by specifying Z₁ and Z₂, which correspond to a range of possible Z values. If Z₁ and Z₂ are specified and a residual is generated with a higher or lower Z, the residual will not be scored in the F8 tally.

The FT8 RES capability is particularly useful with the eighth LCA card entry, NOACT. When NOACT = -2 on the LCA card, the source particle immediately collides in the source material. All subsequent daughter particles then are transported without further collision, as if in a vacuum. The F8 tally with an FT8 RES special tally treatment is then simply the distribution of nuclides resulting from a single collision.

The following input files model a 1.2-GeV proton source having a single collision with ²⁰⁸Pb.

```
Test of p(1.2GeV)+Pb(208)
1 1 -11. -1 imp:h 1
2 0      1 imp:h 0

1 so .01

mode h n
sdef par h erg=1200 vec 0 0 1 dir 1
m1 82208 1
phys:h 1300 j 0
phys:n 1300 3j 0
nps 10000
f8:h 1
ft8 res 1 99
fq8 u e
lca 2 1 1 23 1 1 0 -2 0
```

These data are plotted in Fig. 5, with MCNPX using the tally plotter and the execute line command

MCNPX Z ,

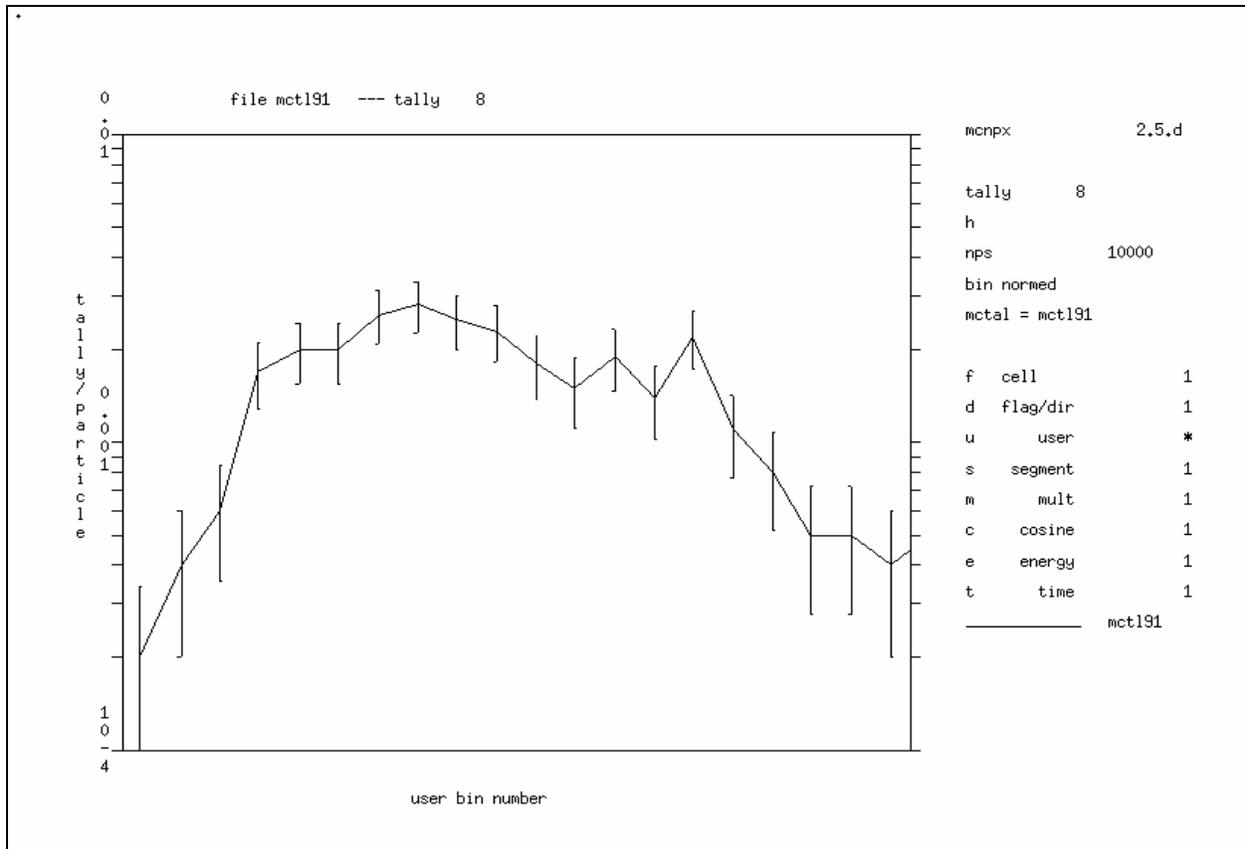


Fig. 5. Residuals for $_{81}\text{Tl}$ isotopes 189 to 201 from 1.3-GeV protons on $^{208}_{82}\text{Pb}$.

where the command file, COM91, is

```
rmctal=mct191
tally 8 free u xlim 81189 8120 ylim .0001 .01 .
```

5.0. OTHER INPUT FILE EXTENSIONS

- Logarithmic interpolation on input cards,
- Auxiliary input files (READ),
- HISTP file size control (HISTP),
- DXTRAN improvements (DBCN), and
- PTRAC file for all particles and for coincidence counting (PTRAC).

5.1. Logarithmic Interpolation

Logarithmic interpolation is allowed on all input cards where lists of numbers are given. It is similar to the IJMR interpolation. For example,

```
E0 1.e-3 6log 1.e4
```

is interpreted as

```
E0 .001 .01 .1 1 10 100 1000 10000 .
```

5.2. Auxiliary Input File and Encryption

The MCNPX READ card enables

- the reading of parts of the input file from other (auxiliary) files,
- the suppression of the printing of the auxiliary input files to shorten output files and protect proprietary information, and
- the encryption of auxiliary input files to protect proprietary information.

The READ card may appear anywhere after the title card of an MCNPX input file but not in the middle of a card continuation.

5.2.1. Reading from an Auxiliary File

```
READ      FILE = filename
```

will cause input from the file “*filename*” to be inserted after the READ command in the MCNPX input deck. Unlike most MCNPX input cards, there may be as many READ cards and auxiliary input files as desired.

5.2.2. Suppressing Input Printing

```
READ      NOECHO
```

will suppress printing of the input cards following the READ card. The echoing of input cards is resumed with

```
READ      ECHO .
```

Because the default of the READ card is ECHO, the echoing also will resume when the next READ card is encountered without the NOECHO command.

The echoing of the input cards also is resumed when an “end of file” is encountered.

```
READ      FILE = filename      NOECHO
```

causes the input from the auxiliary file, *filename*, to be suppressed. After the file *filename* is read, input transfers back to the input file with the READ card and printing is no longer suppressed.

5.2.3. Encryption of Input

A simple encryption scheme is available in MCNPX. The encryption capability can be used to protect proprietary designs of tools and other systems modeled with MCNPX. To read an encrypted file,

```
READ      DECODE password FILE = filename .
```

The encrypted input file will not be echoed, and many default print tables are turned off (and cannot be turned back on) to protect the data in the encrypted file.

To write an encrypted file,

```
READ      ENCODE password FILE = filename .
```

The encryption capability is localized in subroutine ENCRYPT. The MCNPX scheme is very simple; therefore, it protects nothing. To protect input, the subroutine should be modified to a more sophisticated scheme known only to those producing the data and only executable MCNPX versions should be provided to users of the encrypted files.

5.3. HISTP File Size Control

The HISTP card controls the writing of information to an external file for analysis by the HTAPE3X program. HISTP can take two different argument types:

```
HISTP -lhist icl1 icl2 icl3 .
```

lhist is the parameter that controls the number of words written to a *histp* file. Once this limit is exceeded, a new file will be written with the name *histpa* and the incrementing of the name will continue until all particles are run. lhist must be entered as a negative number and may appear anywhere on the card. The default value of lhist is 500,000,000 words.

icl₁, icl₂, ... are cell numbers. If no icl value is present, all events will be written to *histp*. The user may enter as many icl values as needed, and only events within these cells will be written to *histp*.

Example:

```
HISTP -100000 5 6 3 10 .
```

Each *histp* file will contain a maximum of 100,000 words. Only events within cells 3, 5, 6, and 10 will be written to the *histp* file.

```
HISTP
```

By default, each *histp* file will contain a maximum of 500,000,000 words (which virtually ensures that only one file will be written). All events in all cells will be written to the file.

Note: writing *histp* files during multiprocessing is still under development.

5.4. DXTRAN Improvements

5.4.1. Detectors with Model Physics (Isotropic Approximation)

All collisions producing neutrons and photons now contribute to DXTRAN and point detectors, including model physics interactions. When the secondary neutron/photon angular scattering distribution function is unknown (generally the case for model physics), isotropic scattering is assumed (poor approximation). Although the extension to higher energies often is approximate, energy bins for the point detector tally can identify what portion of the tally is coming from high energies. Further, this approximation is superior to neglecting charged-particle and high-energy neutron collisions altogether.

5.4.2. Detector/DXTRAN Underflow Control (DBCN)

DXTRAN and point detector contributions are based on the next-event estimator that makes contributions of

$$W \times p(\mu) \times \exp(-\lambda) / 2\pi R^2 ,$$

where

W = particle weight,

$p(\mu)$ = the density function for scattering to the detector or DXTRAN sphere,

R = the distance from collision to the detector or DXTRAN sphere, and

λ = the attenuation factor, namely the sum of total macroscopic cross sections times the track length for each material region crossed between the collision and detector or DXTRAN sphere.

In MCNP4C, if $\lambda > 80$, then $\exp(-\lambda) = 0$ and the score is terminated as “underflow in transmission.” These small contributions are truncated—that is, they are neglected—which biases answers by omitting them. Generally, they are insignificant to the final answer, but in some cases, the underflow contribution is significant and needed. When DXTRAN spheres or point detectors are used to get tally contributions for generating weight windows, sometimes these underflow contributions cannot be neglected.

It is possible to specify the underflow limit with the sixth entry on the DBCN card. The default is 80, but values between 50 and 200 are accepted.

If DXTRAN/detector underflow is significant in the calculation, serious problems generally exist, such as not sampling enough collisions near the detector. The underflow limit should be changed only with extreme caution.

5.5. PTRAC for All Particles and for Coincidence Counting

5.5.1. PTRAC for All Particles (PTRAC)

The PTRAC capability of writing particle tracks to a file for post-processing has been extended to include all particle types and provides appropriate information for all model collision/bank events.

5.5.2. PTRAC Capture File for Coincidence Counting (PTRAC)

The FT8 CAP coincidence capture tallies may be written to a PTRAC file for further analysis by auxiliary codes. A PTRAC file is created with the following MCNPX input file (INP) input card:

PTRAC *EVENT = cap* *FILE = asc* .

Either an ascii (text) file (*FILE = asc*) or a binary file (*FILE = bin*) may be created. The default is a binary file.

For *EVENT = cap*, most of the standard PTRAC capabilities are bypassed (for speed) and the data written to each line (or binary file record) are very different from the usual PTRAC data.

5.5.2.1. History Information on PTRAC File

For binary files, the entries on each line are

NPS Time Cell .

For ascii files, the entries on each line are (format: i10,1p1e15.5,2i8)

NPS Time Cell Source ,

where

- NPS = the particle history number,
- Time = the time from source event to analog capture in any FT8 cap tally,
- Cell = the cell in which analog capture occurred, and
- Source = the source particle number of a given history.

For example, after the usual PTRAC header, the capture events would be recorded as

NPS	Time	Cell	Source
1	4.5e01	22	4
1	0.0e00	0	3
1	2.6e02	-22	2
1	3.5e02	-22	2
1	1.5e00	23	2
1	0.0e00	0	1
3	0.0e00	0	2
3	0.0e00	0	1

In the previous example, source history 1 (NPS = 1) had four spontaneous fission neutrons (4, 3, 2, 1 in the Source column). The fourth (Source 4—numbering is done as in the MCNPX bank: last in, first out) was captured in Cell 22 at Time = 45 shakes after the source spontaneous fission. The third (Source 3) was not captured (Time = 0.0, Cell = 0). The second (Source 2) caused an induced fission—or possibly several induced fissions—as flagged by the negative cell number. Captures in Cell 22 were at 260 and 350 shakes for these neutrons from induced fission (from the second neutron from a spontaneous fission). The second spontaneous fission neutron

was captured in cell 23; this neutron must have been a branch [after an (n,2n) split, perhaps] that did not undergo fission. The final (first, Source 1) spontaneous fission neutron was not captured.

The second history (NPS = 2) is a spontaneous fission of multiplicity zero; thus, no history 2 exists.

The third source particle history is a fission that results in two fission neutrons (Source = 2, Source = 1), neither of which is captured.

For binary files (*FILE = bin*), only three words per record are written. In the fourth column, "Source" is omitted.

5.5.2.2. Changing the Name of the PTRAC File

The PTRAC file name may be changed on the MCNPX execution line,

```
mcnpX      ptrac = filename ,
```

and the file name will be altered if an old file by that name already exists. For example, if file *ptraca* was the last PTRAC file, then the created PTRAC file would be *ptracb*.

5.5.2.3. Possible Future Extensions of the PTRAC Capture Option

Many standard PTRAC capabilities are missing from the PTRAC capture tally output file capability. If desired, these capabilities could be added and could include nearly all of the remaining PTRAC options: BUFFER, MAX, MEPH, WRITE, other EVENTS, FILTER, particle type, NPS, cell, surface, tally, and VALUE.

6.0. GRAPHICS

MCNPX has the following geometry, tally, and cross-section plotting extensions:

- mesh tallies (tally grid superimposed over geometry) plotted within MCNPX;
- two-dimensional (2D) color contour plots for lattice and radiography tallies;
- enhanced color geometry plots;
- i,j,k lattice indexing in geometry plots;
- geometry plot of WWG superimposed mesh;
- proton and photonuclear cross-section plots; and
- pause command for tally and cross-section plots.

6.1. Color Contour Plots for Mesh Tallies, Radiography Tallies, and Lattice Tallies

Tally output, including mesh tallies, radiography tallies, and lattice tallies, may be plotted as 2D color contour plots. Mesh tallies also can be plotted as superimposed over problem geometries. All of these plots are done in MCNPX without the need of auxiliary post-processing codes. The plots can be made either at the end of a calculation or while a calculation proceeds using the MPLOT card.

The following combinations are available:

Post-processing, MCNPX Z option, RMCTAL = <mtal filename>
 Mesh tallies, radiography tallies, lattice tallies, and all other tallies

Post-processing, MCNPX Z option, RUNTPE = <runtpe filename>
 Radiography tallies, lattice tallies, and all other tallies
 In the PLOT mode mesh tally contours superimposed over problem geometries

Run-time plotting: all of the above combinations are available during a run with the MPLOT input file card.

6.1.1. User Interface for Contour Tally Plots

Mesh tally, radiography, and lattice tally contour plots may use all of the usual MCNPX tally plot (MCPLOT) commands. The FREE and CONTOUR commands have the following extensions.

6.1.1.1. Free Command

The MCPLOT free command is

```
FREE X[Y] [nxm] [all] [noall] .
```

For mesh tallies,

```
FREE ij ,
FREE jk , and
FREE ik
```

are used, where i,j,k refer to the CORA, CORB, and CORC mesh tally dimensions.

For radiography tallies,

```
FREE SC
```

is used to make a contour plot of the s - and t - radiography axes.

For lattice tallies, i,j,k , refer to the i,j,k lattice indices.

If the lattice is fully specified, e.g.,

```
fill=-2:2 -2:2 0:0
2 2 2 2 2
2 2 1 1 2
2 1 1 1 2
2 1 1 2 2
2 2 2 2 2 ,
```

then the [nxm] entries are not needed. If the lattice is not fully specified, e.g.,

```
fill=2 ,
```

then the i and j dimensions must be given with the [nxm] entries, e.g.,

```
FREE ik 20x10 FIX j=15 .
```

The FIX command has its usual meaning, namely that the $j=15$ slice of the full i,j,k lattice will be used.

The “all” and “noall” keywords specify if the minimum and maximum contour range should be taken from all of the tally bins (“all”) or just from those of the FIXED command slice (“noall”—default).

One-dimensional mesh, radiography, and lattice tallies are also possible simply by giving the free dimension on the FREE command:

```
FREE i FIXED j=10 FIXED k=12 .
```

Again, for lattice tallies that are not specified fully, the [mxn] dimensions must be provided. Mesh and radiography tallies are always specified fully, so [mxn] is never required for them.

6.1.1.2. Contour Command

The MCPLLOT contour command is

```
CONTOUR [cmin cmax cstep] [command] [command] .
```

All entries are optional. The [cmin cmax cstep] entries are the minimum, maximum, and step values for contours. The [cmin cmax cstep] entries are numbers and must appear together. The other commands may appear anywhere after the CONTOUR command and are

%	interpret step values as percentages. The default is 5 95 10 %;
pct	interpret step values as percentages. The default is 5 95 10 %;
lin	interpret step values as absolute values of contour levels;
log	contour levels logarithmically spaced between cmin and cmax, with cstep values in between;
all	contours normalized to min and max values of entire tally;
noall	contours normalized to min and max values of (FIXED command) contour slice;
line	draw lines around contours (default);
noline	do not draw lines around contours;
color	make color contour plot (default); and
nocolor	no color; draw line contours only.

Examples:

```
CONTOUR 5 95 10 % line color .
```

Ten contour lines will be at 5%, 15%, ..., 95% of the maximum value. Lines will be drawn around the colored contours, as shown in Fig. 6. The default setting is

```
CONTOUR 1e-4 1e-2 12 log .
```

Twelve contour lines will be logarithmically spaced between tally values of 1e-4 and 1e-5.

6.1.2. Mesh Tally Contour Plot Example

Mesh tallies may be plotted either in the MCNPX tally plotter (MCPLLOT) from MCTAL files or superimposed over geometry plots in the geometry plotter (PLOT) from RUNTPE files.

6.1.2.1. MCPLLOT Mesh Tally

Figure 6 shows a mesh tally of a critical configuration of seven identical barrels of fissionable material. The mesh tally is generated from an MCTAL file in the MCPLLOT tally plotter.

The input file for this problem is

```

cylinders containing critical fluid in macrobody hex lattice
1 1 -8.4      -1      u=1      imp:n=1
2 0           -2      u=1      imp:n=1
3 2 -2.7      -3 1 2  u=1      imp:n=1
4 3 -.001     3       u=1      imp:n=1
10 3 -.001    -6 lat=2 u=2      imp:n=1 fill=-2:2 -2:2 0:0
                                2 2 2 2 2
                                2 2 1 1 2
                                2 1 1 1 2
                                2 1 1 2 2
                                2 2 2 2 2
11 0          -8              imp:n=1 fill=2
50 0          8              imp:n=0

1 rcc 0 0 0 0 12 0 5
2 rcc 0 12 0 0 8 0 5
3 rcc 0 -1 0 0 22 0 6
6 rhp 0 -1 0 0 22 0 9 0 0
8 rcc 0 -1 0 0 22 0 30

m1      1001 5.7058e-2  8016 3.2929e-2
        92238 2.0909e-3  92235 1.0889e-4
m2      13027 1
m3      7014 .8 8016 .2
c
fc14 total keff in each element
f4:n (1<10[-2:2 -2:2 0:0]<11)
fq4 f m
sd4 1 24r
f14:n (1<10[-1 1 0]) (1<10[0 1 0])
        (1<10[-1 0 0]) (1<10[0 0 0]) (1<10[1 0 0])
        (1<10[0 -1 0]) (1<10[1 -1 0]) t
fq14 f m
sd14 1 7r
tf14 4
fm14 (-1 1 -6 -7)

```

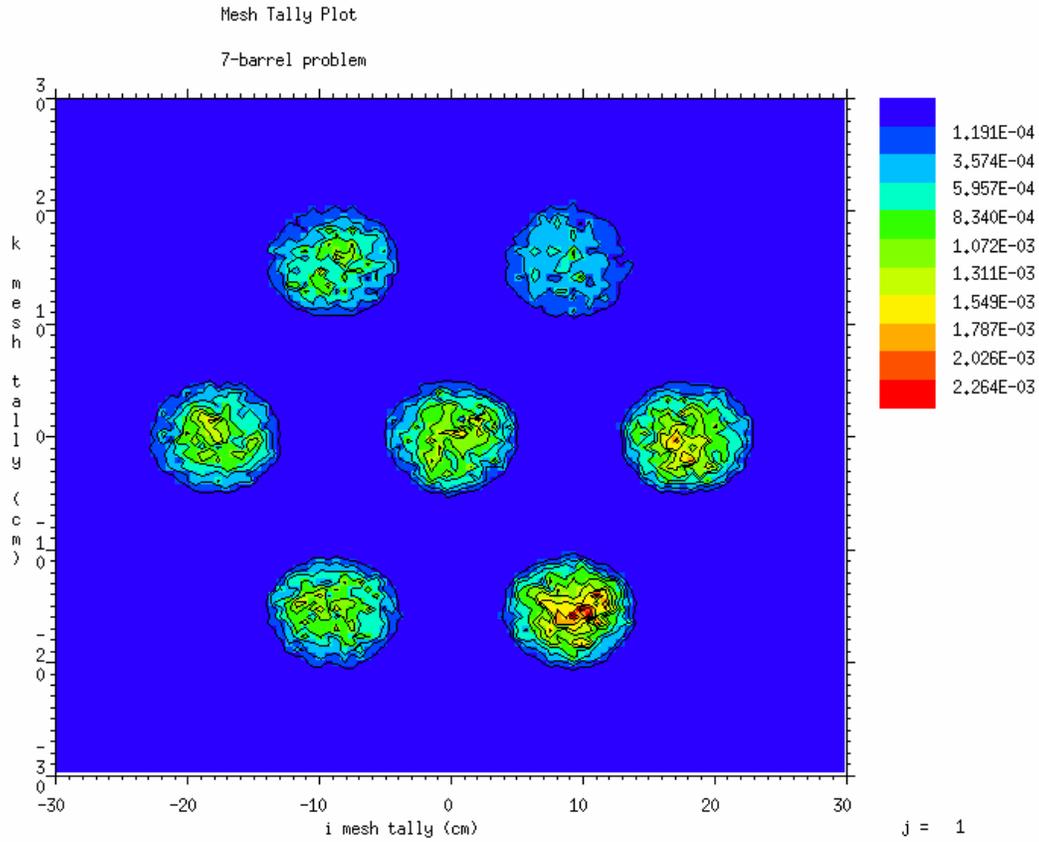


Fig. 6. Mesh tally of barrel geometry.

```

print -160
prdmp 2j 1
kcode 1000 1 10 50
ksrc 0 6 0 18 6 0 -18 6 0 9 6 15 -9 6 15 9 6 -15 -9 6 -15
tmesh
rmesh12
cora12 -30. 99i 30.
corb12 0. 12.
corc12 -30. 99i 30.
endmd
    
```

The plot command is

```
mcplot> tal 12 free ik .
```

The geometry is shown in Fig. 7.

6.1.2.2. Superimposed Geometry Plot Mesh Tally

Figure 8 shows the mesh plot superimposed over the geometry plot. The MCNPX Z option is used, and the commands are

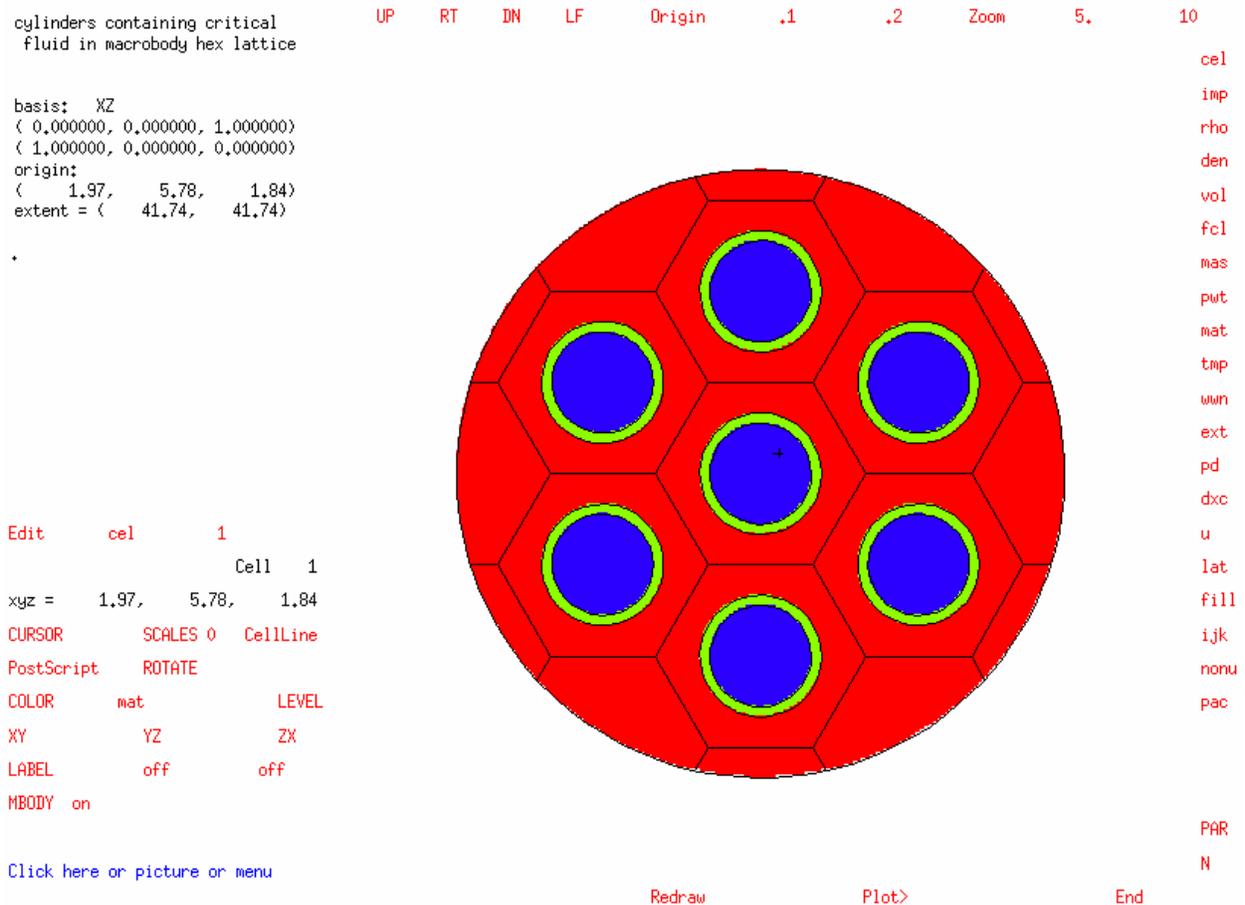


Fig. 7. Geometry of the seven-barrel problem.

```
MCNPLOT> RUNTPE=<runtp filename>
MCNPLOT> PLOT
PLOT> py 4 ex 40 or 0 4 0 la 0 1 tal12 color on la 0 0 con 0 100 % .
```

After the PLOT command, the MCNPX interactive geometry plotter pops up. If the PLOT> button (bottom center) is clicked, then the above command after the PLOT> prompt can be entered. Alternatively, the mesh tally superimposed on the geometry can be viewed by clicking buttons of the interactive tally plot. These options are described in Section 6.1.2.3.

Each outer barrel is expected to have the same source and flux distributions and that the center barrel should have a higher value. However, the mesh tally shows that the barrels do not have the expected distribution. The asymmetric distribution is a known Monte Carlo deficiency and arises in all Monte Carlo codes, including MCNP4C, MCNP5, and MCNPX: eigenvector fluxes generally are converged falsely in eigenvalue problems of critical systems. It is evident that the mesh tally is useful in assessing such deficiencies.

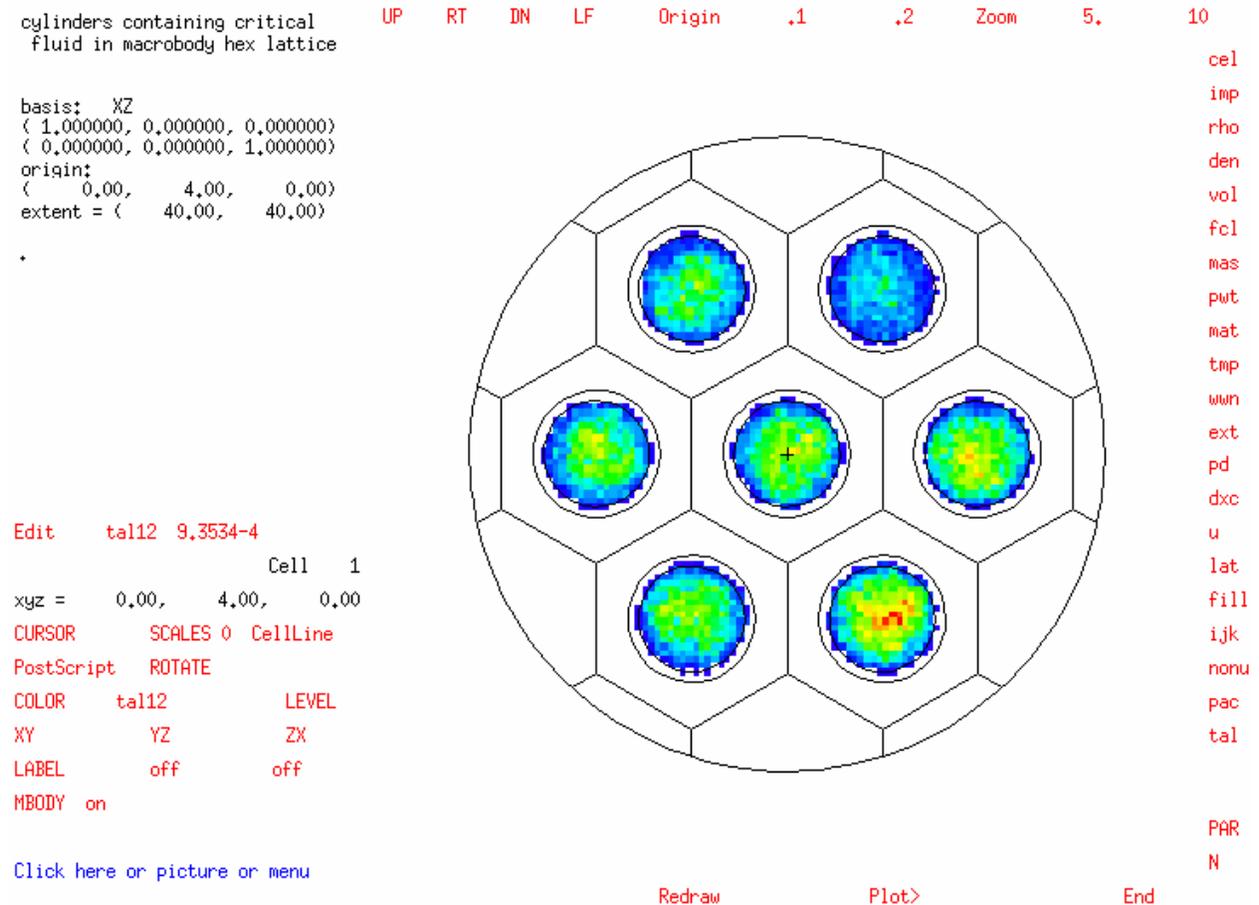


Fig. 8. Mesh plot superimposed on geometry plot.

During the course of a calculation, an MPLOTT card in the INP file can be used to plot the mesh tallies. The plot of Fig. 8 would be achieved with the following MPLOTT card:

```

mplot freq 3000 plot ex 40 py 4 la 0 1 tal12.1 color on la 0 0
cont 0 100 pct

```

The “freq 3000” command causes a plot to be made every 3000 histories. The “plot” command then transfers plotting from the tally plotter to the geometry plotter. The remaining commands are described in Section 6.1.2.3.

When a calculation is completed, the mesh tallies may be plotted as superimposed over geometries using the MCNPX Z option. Only RUNTPE files can be used; MCPLOT files cannot be used because they do not contain the geometry information. The RUNTPE file may be specified either in the execution line,

```

MCNPX Z RUN=<runtp filename> ,

```

or the RUNTPE file may be specified in the usual way anytime when doing tally plots:

```
MCNPX      Z
mcplot>    run=<runtp filename> .
```

Then to get the mesh tallies, the geometry plot mode must be requested:

```
mcplot>    PLOT .
```

At this time, the interactive geometry plotter screen will pop up and commands may be entered either interactively or in command mode by striking the PLOT> button in the bottom center of the screen.

The mesh tally boundaries also may be plotted by cycling through the CellLine options in the interactive geometry plot or by using the command mesh = 6 or mesh = 7 plot commands (Section 6.1.2.3).

6.1.2.3. *Commands for Superimposed Geometry Plot Mesh Tally*

To plot a mesh tally superimposed over a geometry plot, the geometry first must be specified in the usual manner. For the geometry of Fig. 2, the plot commands are

```
PLOT> or 0 4 0 py 4 ex 40 la 0 0 .
```

The same geometry can be viewed by using the Zoom, Origin, XZ, and LABEL interactive buttons.

Next, the tally must be selected as the “Edit” quantity. In the command mode, the only method is to select the tally as the label quantity, transfer the label to the color quantity, and then turn the labels back off:

```
PLOT> la 0 1 tal12.1 color on la 0 0 .
```

Note that only mesh tallies will be recognized. If multiple mesh tally bins exist, e.g.,

```
rmesh11:h flux popul ,
```

then the number after the decimal indicates which bin. In this case, tal11.1 refers to the “flux” mesh tally and tal11.2 refers to the “popul” mesh tally.

Interactive plot buttons can be used to achieve the same result. First, the mesh tallies must be made the “Edit” quantity by clicking the last of the buttons in the far-right column of the screen.

Click	tal	(make mesh tallies the “Edit” quantity),
Click	N	(cycle through available mesh tally numbers), and
Click	IP	(cycle through mesh tally bins).

The “Edit” quantity, e.g., tal12.1, now has been specified. Next, change the color parameter (default = “mat”), by clicking COLOR twice.

Click	COLOR	(will change “mat” to “off”),
Click	COLOR	(will change “off” to the “Edit” quantity, “tal12.1”), and
Click	Redraw	(bottom center button—to make new picture).

Two other commands are also useful: mesh and contour.

The actual mesh tally grid can be displayed by clicking “CellLine” and cycling through the options to get either “MeshTaly” (which draws mesh tally grid lines over the plot) or “MT+Cell” (which draws mesh tally grid lines and cell surface lines over the plot). In the command prompt mode, this is done with

```
PLOT>      mesh = 6          (mesh tally grid lines)
```

or

```
PLOT>      mesh = 7          (mesh tally grid lines plus cell surface lines) .
```

The contour levels can be adjusted using the contour command. No interactive button is available for this; thus, to get from interactive to command mode, either the “Click here or picture or menu” (bottom left of interactive screen) or “PLOT>“ (bottom center) must be struck. The contour command is

```
CONTOUR  cmin cmax [cstep]  command .
```

The “cmin cmax cstep” entries are the minimum, maximum, and step values for contours. Superimposed geometry mesh tally plots do not use steps: the values are shaded by 64 colors. Thus, the cstep entry is ignored and can be omitted; it is allowed only for consistency with the CONTOUR command in the tally plotter (see Section 6.1.1.2). The “cmin cmax cstep” entries are numbers and must appear together. Once a CONTOUR command is entered, subsequent CONTOUR commands use the previous “cmin cmax cstep” values; thus, only the “command” entry is required. The “command” entry may appear before cmin or after cstep or by itself. “CONTOUR” may be abbreviated simply to “CON” or “CONT”. The allowable entries for “command” are

%	interpret step values as percentages. The default is 5 95 10 %;
pct	interpret step values as percentages. The default is 5 95 10 %;
lin	interpret step values as absolute values of contour levels;
log	contour levels logarithmically spaced between cmin and cmax; and
off	use default: 0 100 % .

The remaining command options for tally plots (“all”, “noall”, “line”, “noline”, “color”, and “nocolor” (see Section 6.1.1.2) make no sense for geometry mesh tally plots and are disallowed. Some examples are

```
cont 0 100 pct
con 5 95 10 %
contour off
cont 1E-4 2 log
```

6.1.3. Radiography Tally Coutour Plot Example

The following example is a radiograph of a 4-cm-radius, 1-cm-thick ^{238}U disc with an embedded 4-mm-void sphere and skew-oriented 1-cm \times 1-cm \times 8-mm box. The input file is

```
Radiography Tally
1 5 -25.0 -1 4 5 imp:p=1
2 0      1 -2  imp:p=1
3 0      2  imp:p=0
4 0      -4  imp:p=1
5 0      -5  imp:p=1

1 RCC 0 0 0 0 0 1 4
2 RPP -100 100 -100 100 -100 100
4 SPH 3 0 .5 .4
5 BOX -1 1 .1 .6 .8 0 -.8 .6 0 0 0 .8

mode p
nps 100 5
sdef pos=0 0 -20 axs=0 0 1 rad=d1 ext=0 vec=0 0 1 dir=d2 erg=6
sil 0 .1
sp1 -21 1
si2 -1 1
sp2 -31 1
m5 92238 1
print
prdmp 2j 1
tir5:p 0 0 10 0 0 0 -100 0 100 0
fs5 -10. 99i 10.
c5 -10. 99i 10.
```

The x-y geometry plot of this geometry is given in Fig. 9.

To get the contour plot, run

```
MCNPX      Z      RUNTPE=filename .
```

The contour plots also may be read from a MCTAL file instead of the RUNTPE. When the code gives you the MCPLLOT prompt, enter two dimensions with the free command; for example, S and C:

```
MCPLLOT> free SC .
```

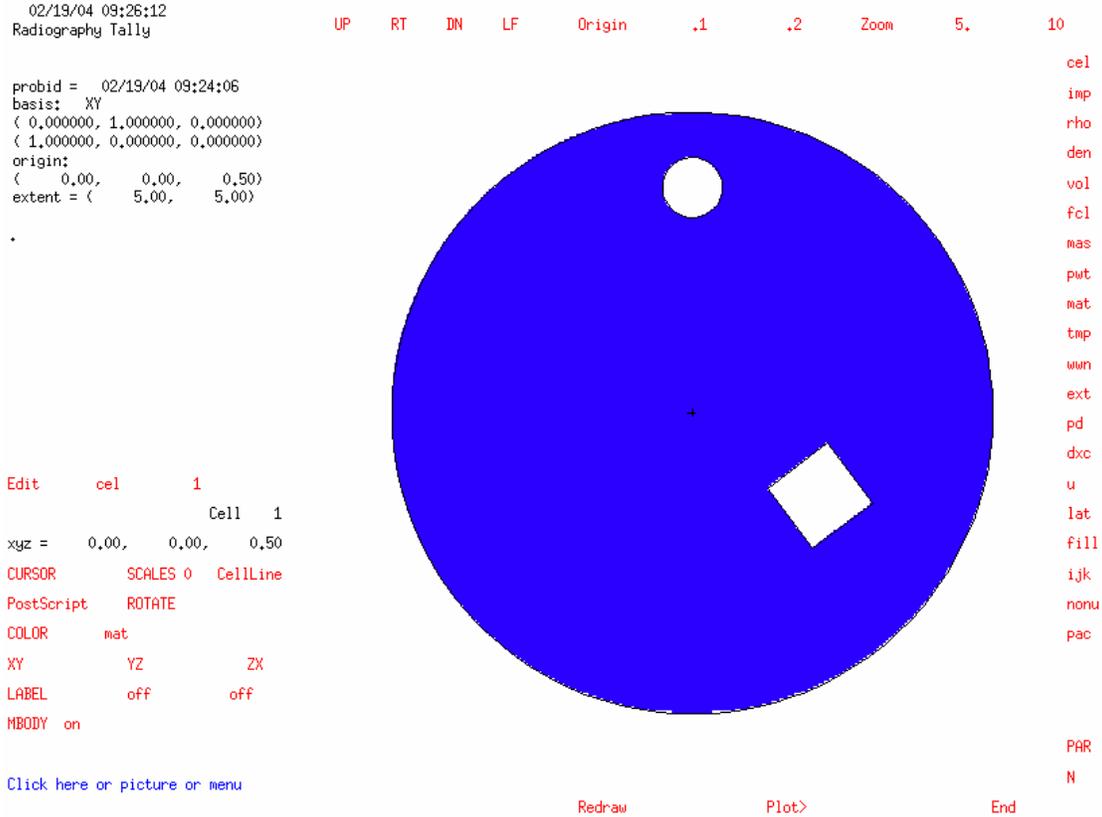


Fig. 9. Geometry plot of radiograph example.

Recall that the tally dimensions are

- F surface/cell/detector F card bin,
- D total/direct or flagged bin,
- U user bin,
- S segment or radiography s-axis bin,
- M multiplier bin,
- C cosine or radiography t-axis bin,
- E energy bin, and
- T time bin.

The results are plotted in Fig. 10. The embedded sphere and box are seen plainly in the disc.

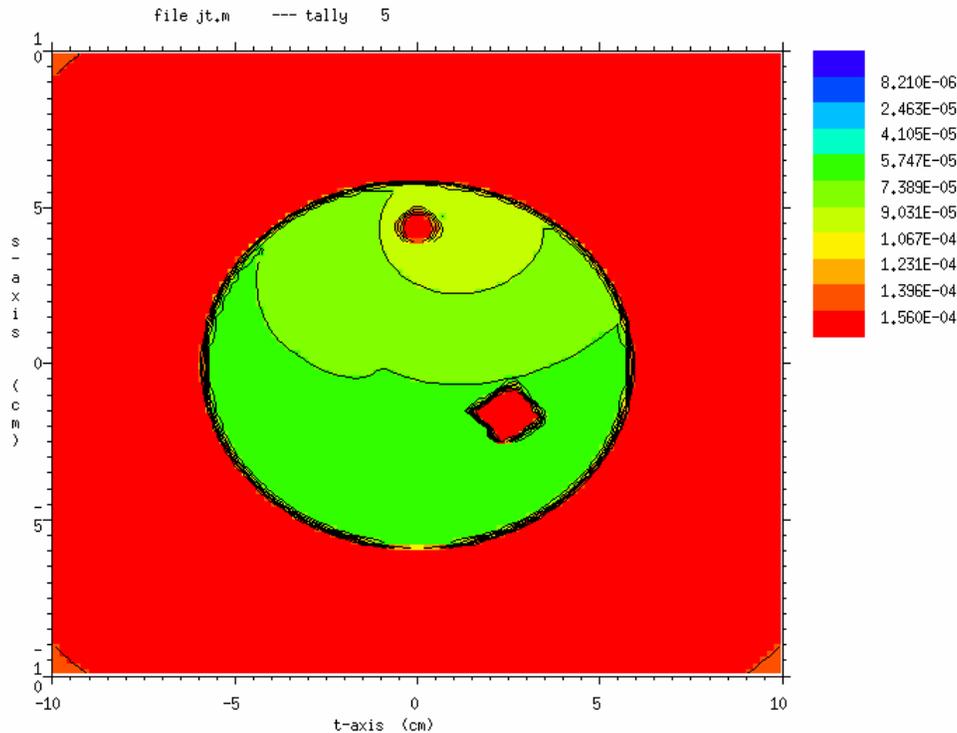


Fig. 10. Scattered photon radiographic image of ^{238}U disc.

6.1.4. Lattice Tally Plot Examples

Lattice tallies also may be plotted as either 1D or 2D contour plots. An example of a lattice tally 1D plot is

```
free i 64x64 fix j = 38 fix k = 30 .
```

This command specifies a 1D lattice tally plot of the cell bins, which should correspond to a lattice tally with 64 “i” index bins, 64 “j” index bins, and at least 30 “k” index bins. With the “k” index set to 30 and the “j” index to 38, the offset into the f bins will be $29 \times 64 \times 64 + 37 \times 64 = 121,152$. The minimum and maximum values will be determined from the 64 “i” bin values included in the plot. If the “j” and “k” indices are not specified, their default value of 1 is assumed, which results in an offset of 0.

An example of a lattice tally 2D contour plot is

```
free ij 10x30 all fix k=60 .
```

This example specifies a 10×30 2D contour plot, which should correspond to a lattice tally with 10 “i” bins, 30 “j” bins, and at least 60 “k” bins. Note that the “k” index is specified using the “fix” command, which sets the offset into the f bins as $60 \times 10 \times 30 = 18,000$. In this case, the contour range is taken from all of the f-bin tally values.

6.1.5. Other Notes and Future Work

A consequence of the mesh tally contour plotting capability is that MDATA files are ignored in continue runs. MDATA files and the auxiliary GRIDCONV code still are supported for the plotting of mesh tallies with other postprocessors, such as MORITZ and TECPLOT. A new MDATA file is written at the end of each initial or continue run.

When using COMMAND files (which use a preselected sequence of MCNPLOT tally plot commands), the “RETURN” command must follow geometry plot commands to revert from the geometry plotter back to the tally plotter.

The future work is as follows:

1. Treat the mesh tallies as regular tallies. Among the many consequences are the following.
 - RMESH, CORA, CORB, CORC, etc., could be anywhere in the input deck (TMESH and ENDMD would be ignored), and all other tally features, such as FM, DE, DF, FC, CF, SF, FU, FT, E, T, EM, and TM, would be enabled and consistent with other tallies; and
 - tally plot mesh tallies (Section 6.1.2.1) could use RUNTPE files and not be limited to MCTAL files.
2. Plot theta and phi values from cylindrical and spherical meshes correctly in tally plots and plot spherical mesh tally grid lines in geometry plots.

6.2. Enhanced Color Geometry Plots: 64-Color Plotting and Shading by Cell Parameters

MCNP4C3 had 10-color plotting; MCNPX has 64-color plotting. Shading of geometry plots may be used for any cell parameter. MCNP4C colored its geometry plots by material only, giving a different color to each material number. MCNPX can color geometry plots by any cell quantity. Each cell can have a different color, or each repeated structure level or universe can have a different color. Logarithmic shading of importances, weight windows, and summary information are automatic. If a superimposed weight-window mesh is used, coloring also may be done by the value of the mesh weight windows.

In the interactive capability, the “SCALES n” button has been moved up two lines (after the cursor) to make room for a larger “COLOR name” button. The default is “COLOR mat”, which colors problem cells by the program material number. This button must be clicked to get “COLOR off” (black and white) and then clicked again to color by whatever parameter is listed after the “Edit” button. For example, in the right margin, click “cel”, which will make the “Edit” quantity “cel”. Next, click “COLOR” so that “COLOR cel” is displayed; on the next plot, the color shades will be determined by program cell number.

For command/prompt plotting, enter

PLOT> label 0 1 rho ;

the color command then must be set such as

PLOT> color on ,

and the coloring will now be by rho, the atom density.

6.3. i,j,k Lattice Index Labeling

The i,j,k lattice indices of repeated structures/lattice geometries may be used as plot labels in geometry plots, as illustrated in Fig. 11.

If the level (LEVEL command or button) is not a lattice cell level, then the indices will be those of the next lattice in a higher level. To get the lattice index labels, choose “ijk” as the “Edit” quantity by clicking “ijk” in the right margin. Then click the send entry after LABEL so that it reads “LABEL off ijk”. For command/prompt plotting, enter “Label 0 1 ijk”.

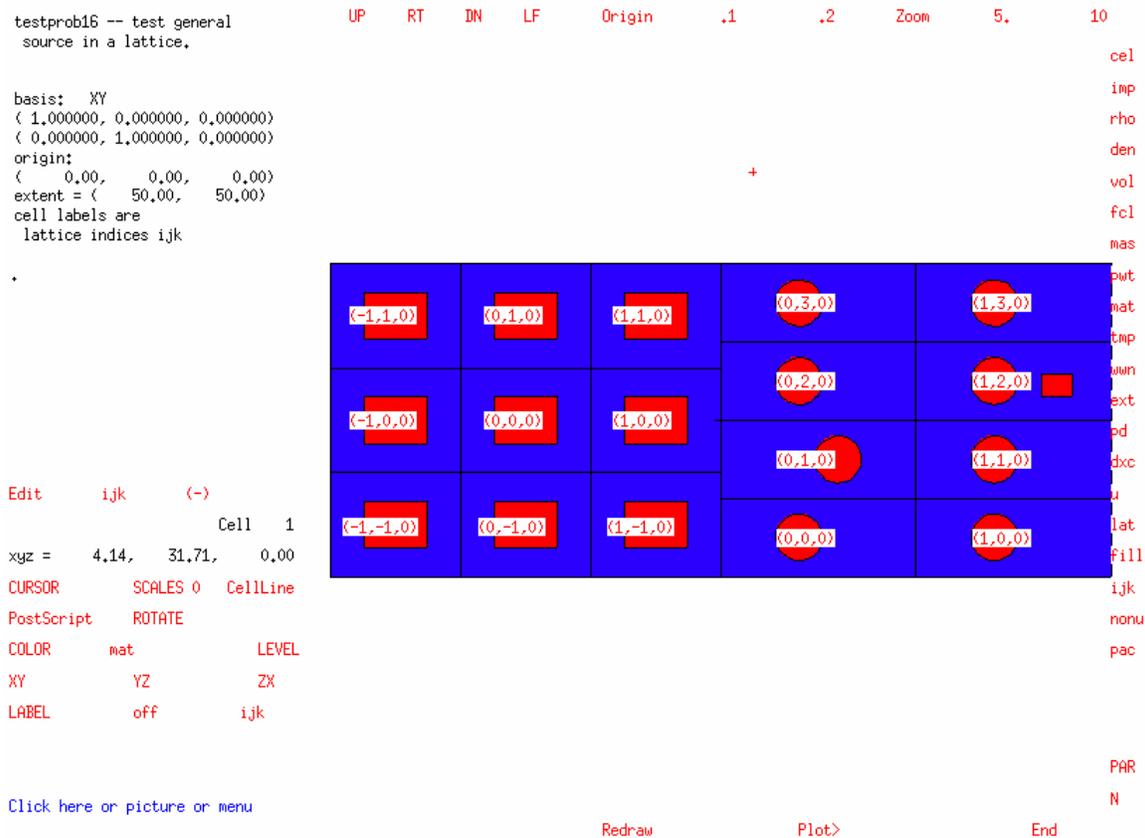


Fig. 11. Lattice indexing in geometry plot.

6.4. Weight-Window-Generator Superimposed Mesh Plots

MCNPX can plot the WWG superimposed mesh specified on the MESH card in an input file. MCNP4C3 and previous MCNPX versions could plot only the weight-window superimposed mesh used in a problem, and a WWINP file had to be provided. In the MCNPX geometry plotter, toggle CellLine for the following options:

No Lines	Plot cells not outlined in black
CellLine	Plot geometric cells, outlined in black
WW MESH	Plot the weight-window superimposed mesh (WWINP required)
WW+Cell	Plot superimposed mesh and cells, outlined in black
WWG MESH	Plot MESH card WWG mesh
WWG+Cell	Plot WWG mesh and cells, outlined in black
MeshTaly	Plot mesh tally boundaries
MT+Cell	Plot mesh tally boundaries + CellLine

The CellLine and No Lines options are always available. WW Mesh and WW+Cell are available only when the WWP card calls for using a superimposed weight-window mesh (fifth entry negative) and a WWINP file is provided. WWG MESH and WWG+Cell are available only when a MESH card is in the input file and when the WWG requests superimposed mesh generation (WWG card second entry = 0). In all cases, the cells may be outlined in black (CellLine, WW+Cell, WWG+Cell) or the cells simply may be colored without outlining (WW MESH, WWG MESH, No Lines).

6.4.1. Geometry Plot of Weight-Window-Generator Superimposed Mesh

MCNPX can plot the WWG superimposed mesh specified on the MESH card in an input file. The following options are available.

0.	No Lines	Plot cells not outlined in black
1.	CellLine	Plot geometric cells, outlined in black
2.	WW MESH	Plot WW mesh (WWINP, WWP 4j -1 required)
3.	WW+Cell	Plot WW mesh (WWINP, WWP 4j -1 required) + CellLine
4.	WWG MESH	Plot WWG mesh (MESH, WWG J 0 required)
5.	WWG+Cell	Plot WWG mesh (MESH, WWG J 0 required) + CellLine
6.	MeshTaly	Plot mesh tally boundaries (RMESH, CORA, etc., required)
7.	MT+Cell	Plot mesh tally boundaries + CellLine

In the interactive MCNPX geometry plotter, toggle CellLine for the above options.

In the command-mode geometry plotter, the option is *mesh = n*, where *n* is the number 0 to 7, as determined by the options list above.

The CellLine and No Lines options always are available. WW MESH and WW+Cell are available only when the WWP card calls for using a superimposed weight-window mesh (fifth entry negative) and when a WWINP file is provided. WWG MESH and WWG+Cell are available only when a MESH card is present in the input file and when the WWG requests superimposed mesh generation (WWG card second entry = 0). In all cases, the cells may be

outlined in black (CellLine, WW+Cell, WWG+Cell) or the cells simply may be colored without outlining (WW MESH, WWG MESH, No Lines).

6.4.2. Example

Input file: *inp10*

Demonstration of WWG Plot

```
1 1 1.0 -1 imp:p 1
2 0      1 imp:p 0
```

```
1 rcc 0 0 0 0 10 0 5
```

mode p

```
sdef sur 1.3 vec 0 1 0 dir 1 erg 100
```

```
m1 1001 2 8016 1
```

```
nps 1000
```

```
f1:p 1.2
```

```
wwg 1 0
```

```
mesh geom=cyl origin=0 -1 0 ref=0 .1 0 axs=0 1 0 vec=1 0 0
```

```
    imesh 6   iints 7   jmesh 12   jints 7   kmesh 1   kints 3
```

Com file: *com10*

```
ex 10 lab 0 0 px 0 mesh 4
```

```
pause
```

```
py 5
```

```
pause
```

```
mcnpX          i = inp10          com = com10    ip .
```

Or, instead of using the command file (with plot commands in command mode), the interactive plotter can be used.

```
mcnpX i = inp10 ip ,
```

click	CellLine	to get WWG + Cell
	label sur	to turn off surface labels
	XY	to get px = 0 view (axial view, Fig. 12)
	Zoom 10	to get 10× magnification (click twice)
	Origin	click in the center of material to center picture
	ZX	to get py = 5 view (radial view, Fig. 13)

The above Com file or plot commands in the command mode generate the two plots shown in Figs. 12 and 13.

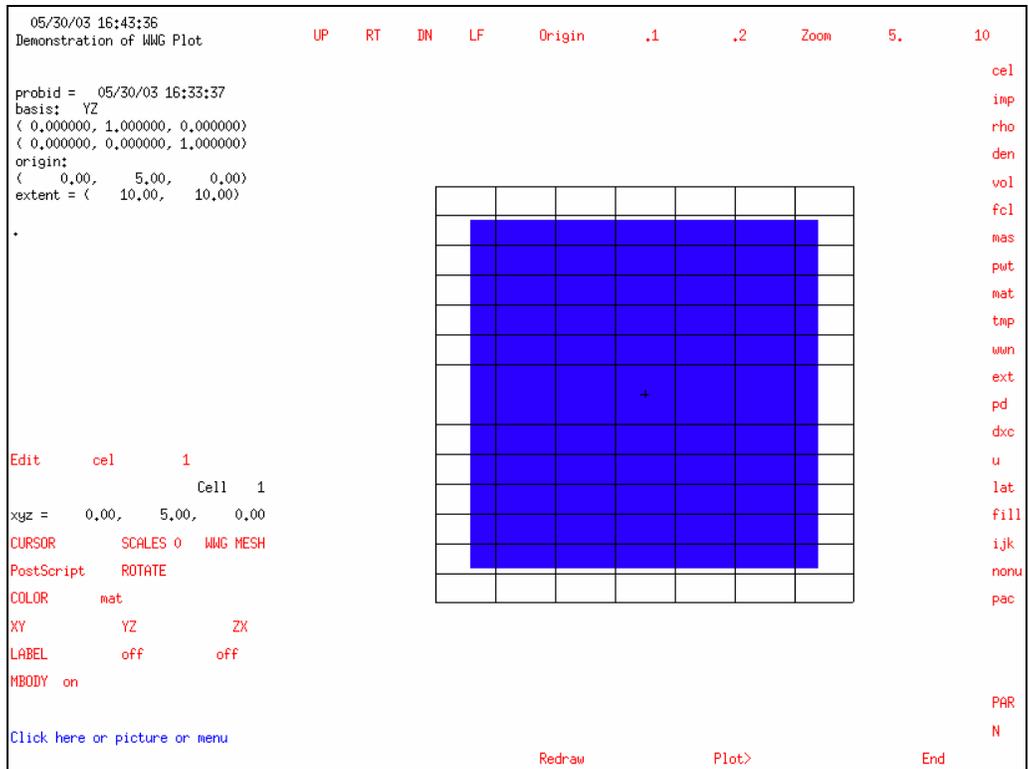


Fig.12. WWG mesh plot, axial view.

6.5. Proton and Photonuclear Cross-Section Plots

6.5.1. Photonuclear Cross-Section Plots

MCNPX can plot photonuclear data, in addition to the photoatomic data of MCNP.

Photoatomic reaction numbers are all negative: -1 = incoherent, -2 = coherent, -3 = photoelectric, -4 = pair production, -5 = total, and -6 = heating. For the MCNPX photonuclear cross-section plotting, the reaction numbers all are positive. The principal photonuclear cross sections are as follows: 1 = total, 2 = nonelastic, 3 = elastic, 4 = heating, and >4 = various reactions such as 18 = (γ, f) . The photonuclear yields (multiplicities) for various secondary particles are specified by adding 1000 times the secondary particle number to the reaction number. For example, 31,001 is the total yield of deuterons (particle type d = 31), 34,001 is the total yield of alphas (particle type α = 34), and 1018 is the total number of neutrons (particle type n = 1) from fission. To find out which reactions are available for a particular nuclide or material, enter an invalid reaction number, such as mt = 99, and MCNPX will list the available photonuclear reactions and the available yields, such as 1018; 31,018; and 34,018. Entering a bad nuclide, xs = 12345.67u, will cause MCNPX to list the available nuclides.

Figure 14 illustrates a photonuclear cross-section plot of the total photonuclear cross section, mt = 1, for material 11 and its constituents, carbon and lead.

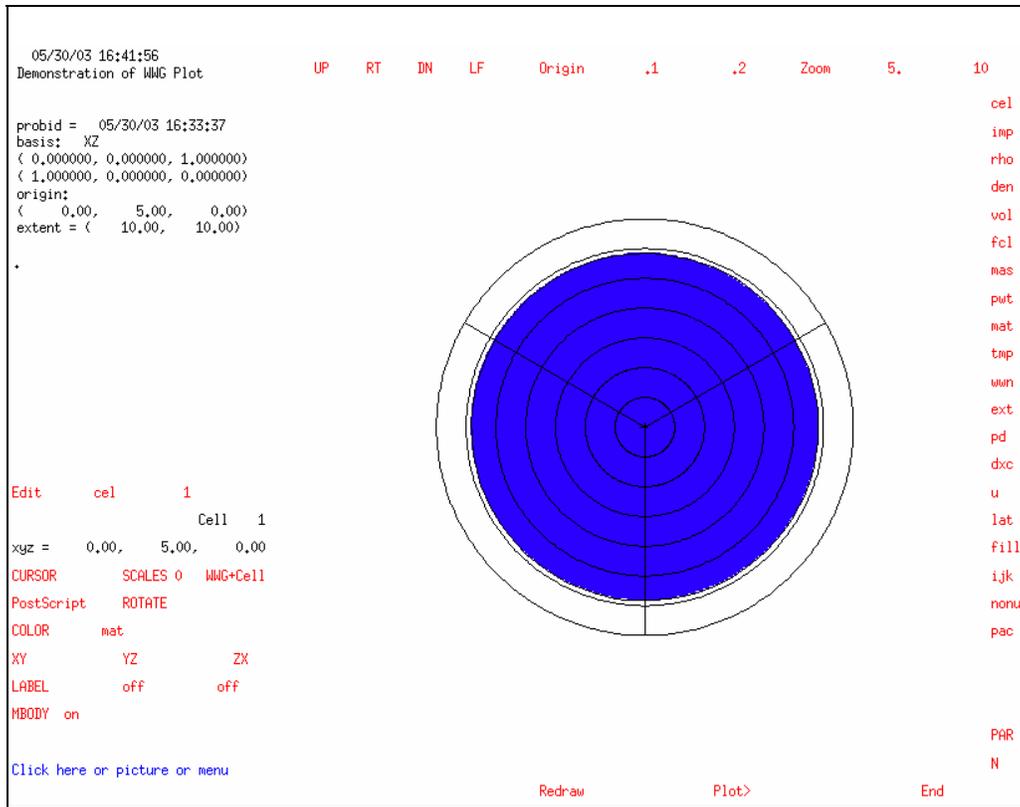


Fig. 13. WWG plot, radial view.

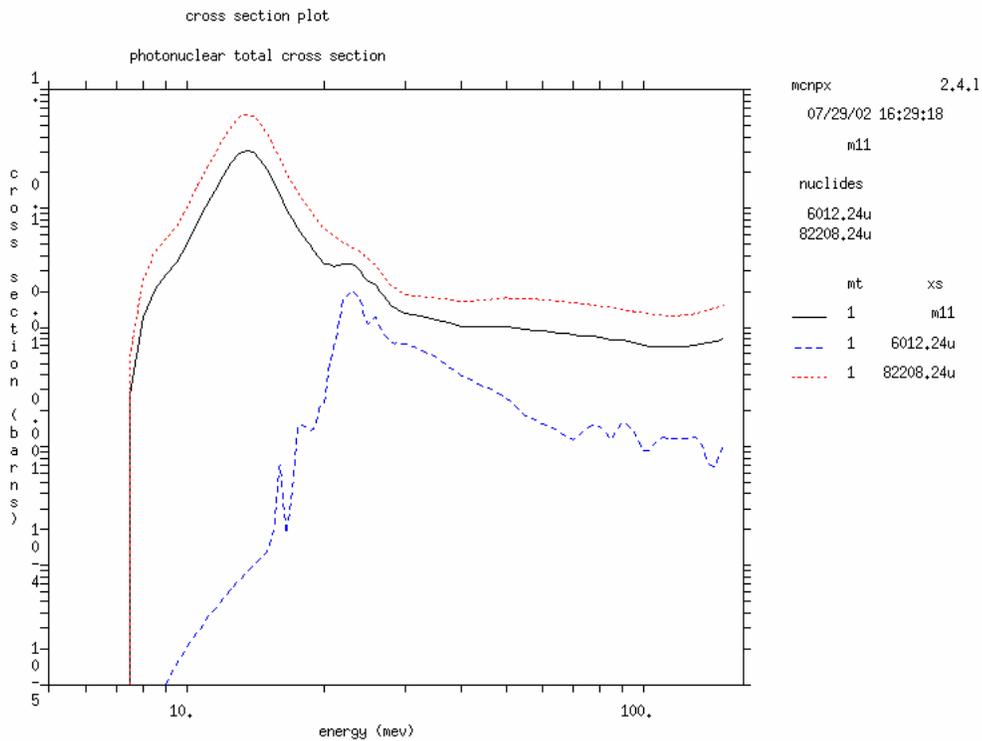


Fig. 14. Photonuclear cross-section plot.

6.5.2. Proton Cross-Section Plots

MCNPX can plot proton cross sections. The reaction numbers are similar to the neutron reaction numbers: all positive. The principal proton cross sections are the following: ± 1 = total, ± 2 = nonelastic, ± 3 = elastic, ± 4 = heating, and >4 = various reactions. On the LA150H proton library, the only available reaction is $mt = 5$ with its multiplicities, 1005; 9005; 31,005; etc. The multiplicity reaction numbers for interaction reaction $mt = 5$ are 1005 for neutrons, 9005 for protons, 31,005 for deuterons, etc. To find out which reactions are available for a particular nuclide or material, enter an invalid reaction number, such as $mt = 99$, and MCNPX will list the available proton reactions and the available yields, such as 1005; 32,001; and 34,002. The proton multiplicity, $mt = 9001$, 9004, 9005, etc., generally is available, along with the total cross-section and heating number, $mt = 1$, $mt = 4$. Entering a bad nuclide, $xs = 12345.67h$, will cause MCNPX to list the available proton nuclides.

6.6. Pause Command

The MCNPX geometry plot *PAUSE* command is extended to tally and cross-section plots. When the word *PAUSE N* is put in a tally plotting the COM input file, the picture will display for *N* seconds. If the command *PAUSE* (without the *N*) is in the COM file, the display will hold until a key is struck.

The reading of the COM file can be interrupted and control of plotting can be returned to the terminal by entering “*quit.*” After each picture is displayed, the message to the command terminal is

Strike any key to continue. Quit returns to interactive mode.

7.0. PARALLEL PROCESSING

- Distributed memory multiprocessing for all particles and energies
- MPI multiprocessing
- Significant speedup of criticality problems run with MPI

7.1. Distributed Memory Multitasking for the Entire Energy Range of All Particles

The entire MCNPX code may be run in parallel using message passing. Table physics problems (i.e., standard MCNP4C3 problems) can be run with threading and/or message passing. Fault tolerance and load balancing are available, and multiprocessing can be done across a network of heterogeneous platforms. Parallel Virtual Machine (PVM) or MPI software can be used.

The parallel message passing capability applies to all particles for their entire energy range and for all physics models.

7.2. MPI Multiprocessing

The MPI parallel communication software is supported by MCNPX. To compile MCNPX with MPI, it is necessary to use the “MPILB” configuration option and provide a path to the MPI

header file. This may not be necessary on some systems if these header files are already in the standard include path:

```
Configure --with-MPILIB[="/path/to/MPI/libraries -lmpich"]
--with --FFLAGS="-I/path/to/MPI/include/files" .
```

To run an MCNPX problem with MPI, simply start the MPI daemon (which typically is running already on most systems) and then start MCNPX using "MPIRUN". An example is

```
mpirun -np 4 mcnpx inp=gwm na=gwm1. ... .
```

MPI is quite different from the PVM, which required knowledge about setting certain links, environment variables, and the PVM console commands. An example of the PVM execution command is

```
mcnpix inp=gwm n=gwm1. tasks=-12 .
```

See "installation notes for building MCNPX with MPI" on the MCNPX documents page at <http://mcnpx.lanl.gov/documents.html>.

7.3. MPI Speedup for Criticality Calculations

Note: The MPI speedup capability speeds up MPI KCODE calculations but also has some collateral consequences for sequential KCODE calculations.

Criticality calculations (KCODE source) will run 10 to 1000 times faster than MCNP4C3 in parallel with MPI multiprocessing. The speedup depends on the number of CPUs and the number of histories per cycle. As the number of CPUs increases above ~8 and the histories per cycle approach ~1M, the speedup increases rapidly from a factor of ~10 to above 1000 with 64 CPUs.

The speedup has been achieved by having the next-generation fission source points on each processor stay on that processor. No longer are the fission source points from all processors combined at the end of each cycle for rebroadcast in the next cycle. The considerable expense of grouping the particles together at each processor rendezvous has been eliminated.

7.3.1. DXTRAN and Detector Tracking Differences

All calculations with DXTRAN and detectors—not just KCODE or parallel calculations—generally no longer track. Answers are still correct, but these next-event estimator problems do not track unless the twenty-first entry on the DBCN card is set to nonzero or the default Russian roulette detector game (DD card) is not played. The tracking difference occurs because the default Russian roulette game no longer adjusts the roulette criteria at the two-hundredth history. The Russian roulette criteria are still set at all tally fluctuation chart intervals, NPD, the fifth entry on the PRDMP card. The default for NPD is 1000 histories for fixed-source problems but is NPD = 1 (at the end of each cycle) for KCODE problems. Thus, a fixed-source problem that previously started playing Russian roulette on next-event estimates at history 200 now waits until history 1000.

7.3.2. User Interface Changes for Both Sequential and Parallel KCODE Problems

The MPI speedup capability has consequences for both sequential and parallel KCODE calculations.

- Tally fluctuation charts are printed only at the ends of KCODE cycles rather than at specific particle intervals.
- The units for the fifth entry of the PRDMP card are changed for KCODE calculations. The fifth entry is NPD, the tally fluctuation chart print interval. For KCODE calculations, NPD is the number of cycles (default = 1).
- KCODE problems with DXTRAN and point detectors are still correct but may not track previous versions if the default Russian roulette game on small scores is played. The tracking difference occurs because the roulette criteria are updated in different places. DXTRAN and detectors using negative DD card entries (to have a constant Russian roulette game criteria) still track.
- Setting the twenty-first entry on the DBCN card to 1 will cause MCNPX to track previous MCNPX versions without the MPI speedup capability:

```
DBCN 20J 1 .
```

7.3.3. User Interface Changes for Parallel KCODE Problems

- The KCODE speedup is available only for negative JTASKS: $tasks = -n \times m$ on the MCNPX execution line. Microtasking/load-balancing (positive JTASKS) calculations use the slower former MCNP4C communication algorithm for KCODE source updating. A warning is issued if $JTASKS > 0$ in a KCODE calculation.
- In rare cases, a subtask may deplete its source particles. Only problem efficiency is affected, and a warning is issued.

7.3.4. Compiler and Operating System Problems for Parallel KCODE Problems

- CTRL-C and quit on a multiple processor MPI run in Linux do not finish writing the OUTP file before MCNPX exits. This failure appears to be an MPI error (possibly feature) in the MPI_FINALIZE call, where the last processor kills all subtasks and the master.
- CTRL-C interrupt does not function properly in Windows 2000 (probably general to all Windows). The user can attempt to quit, but MCNPX will hang and the user will be forced to kill the process through multiple CTRL-C commands.
- The Portland Group pgcc compiler (Version 4.02) will not compile the ANL mpich-1.2.5 properly on a Linux system; however, GCC 3.2.3 will work to build the MPICH libraries.

8.0. COMPILING, CONFIGURATION, AND INSTALLATION

- F90 modularity and dynamic memory allocation
- F90 autoconfiguration
- 64-bit-integer support
- NAG/IBM/INTEL compiler extensions

8.1. F90 Modularity and Dynamic Memory Allocation

The F90 conversion provides improvements in code modularity, standardization of functions such as timing across platforms, and compiler reliability. F90 will run more slowly on some systems. Specifically, we have eliminated equivalences as a means of dynamic storage allocation by using F90 pointers and allocable arrays. We have replaced most common calls with F90 modules. The code will compile in both free and fixed F90 formats.

MCNPX can be modified by patches, and as much of the MCNP4C coding as possible has been preserved so that MCNP4C patches can be applied directly to MCNPX.

Continuing improvements in the F90 structure are ongoing, especially where they concern physics modules that have been brought into the code.

8.2. F90 Autoconfiguration

MCNPX has a unique autoconfiguration build system that allows a variety of compilation options to be executed easily on a large number of platforms. MCNPX supports Linux, Windows PC, Sun Solaris UNIX, HPUNIX UNIX, IBM AIX UNIX, and SGI UNIX.

Test problems and their solution templates are available for all supported systems. The 65 test problems consist of the 42-problem MCNP5 test set supplemented by 23 problems testing MCNPX exclusive features. The test problems on all systems can be run and compared with the solution templates with a single, simple auto-configuration command.

8.3. 64-Bit-Integer Support

MCNPX has been restructured to enable 64-bit integers. MCNP and MCNPX always have had 64-bit floating-point reals, either by use of compiler directives on supercomputers or by double precision on “cheap” computers (most systems). However, the integers have been 4 byte (32 bit) on all but a few supercomputers; 4-byte integers limit the number of histories that can be run to about 2 billion. They also limit the number of cross sections and tallies in a problem because the cross-section data use integer pointers.

With the 64-bit-integer capability, up to 1e18 histories can be run. Memory access problems can be avoided, and nearly all the cross sections and tallies needed can be used.

The print field for the number of histories run in a problem has been increased to 12 digits to accommodate the long runs made possible with parallel processing.

8.3.1. Recompilation Requirements for 64-Bit Integers

The default for MCNPX is still 4-byte integers. The executable versions provided on the MCNPX Beta Test page are all 4-byte integer versions. To use the 64-bit version, it is necessary to

1. recompile with special options and
2. either use Type-1 ascii cross-section tables or rebuild the Type-2 binary cross-section tables with MAKXS using 64-bit integer pointers.

Users who generally recompile their own MCNPX versions and use type-1 ascii cross sections can change to the 64-bit integers rather easily. When configuring, simply use the options

```
--with-FFLAGS=-i8 --with-NOCHEAP .
```

The `--with-NOCHEAP` directive is not available on all systems. If it is not recognized, then add the compile directive

```
--with-FFLAGS=-i8
```

and remove `--DCHEAP=1` from `src/mcnp/mcnpf/Makefile.h`.

The 64-bit integer capability is unavailable on PCs. The `--i8` compile option is not available on the CVF F90 compiler and possibly other compilers. The 64-bit integers will increase the size of the code.

8.3.2. Additional Notes

The 64-bit-integer capability was an extensive change to MCNPX because it affected most F90 “kind” specifications. We also eliminated all “REAL” declarations where floating point variables went to different default lengths (usually 32 bit) on various systems. A consequence is that real variables are all 64 bit unless some other length is required for interfaces to plotting or interrupts or other special purposes. The tracking between different compilers and platforms is now more consistent. Finally, this capability made extension to new compilers and platforms easier (see Section 8.4).

8.4. NAG/IBM/INTEL F90 and Compiler Extensions

MCNPX runs on a wide variety of platforms and operating systems by using more standard F90 constructs and some fairly extensive code and autoconfiguration changes. In particular, it runs on the G5 OS X system, using the NAG 4.2 compiler for the Apple Power Mac G5. MCNPX also runs on this platform with the IBM compiler.

The NAG compiler passes the MCNPX SGI-UNIX test suite on the Mac with “-O1” optimization. The IBM compiler passes with “-O2” optimization and is 17% faster. A trial version of the IBM compiler is available from <http://www.ibm.com/>; see “support & downloads - -- trials & betas A-Z --- XL Fortran.” No MCNPX parallel capability is available yet for the NAG compiler.

MCNPX can use the Intel f90 and C compilers. Thus, on Linux, both the Intel and Portland Group compilers can be used. On Windows, both the Intel and Compaq Digital Fortran (CDF) or earlier Digital Visual Fortran (DVF) f90 compilers can be used. The Windows Intel executable runs the MCNPX test suite an average of 24% faster than the CVF executable. Therefore, the Intel compiler is the default for compilation with Windows PC.

The four configure options on Windows are

Configure	(Build with the Intel compiler)
Configure CVF	(Build with the CVF compiler)
Configure I8	(Build with 8-byte integers)
Configure MPI	(Build the MPI version)

9.0. SUMMARY OF MCNPX CAPABILITIES SINCE MCNP4B (BY VERSION)

The extensions of MCNPX beyond MCNP4B are listed according to version release; the initials of the principal developers are shown in parentheses.*

MCNPX 2.5.f (February 2005)

- Mesh tally plots without auxiliary codes Mesh tallies (tally grid superimposed over geometry) plotted within MCNPX (JSH/GWM);
- PHT with Variance Reduction (JSH/GWM);
- Windows Intel Compiler Support (GWM);
- Improved Photonuclear Model Data (FXG);
- FT8 Capture Tallies with Time Gating (JSH)
- Improved or User Specified Fission Multiplicity Constants—FMULT (JSH)
- Translated Sources with Dependence (GWM)

MCNPX 2.5.e (February 2004)

- 2D color tally contour plots, including lattices and radiography (GWM);
- significant speedup of criticality problems run with MPI (GWM/NAC);
- 64-bit-integer support (GWM);
- NAG/IBM/INTEL compiler extensions (GWM); and
- photon Doppler broadening (from MCNP5) (AS).

* Kenneth J. Adams (KJA), Nate A. Carstens (NAC), Leland L. Carter (LLC), Jean-Christophe David (JCD), Skip Egdorf (HWE), Thomas M. Evans (TME), Jeffrey A. Favorite (JAF), Franz X. Gallmeier (FXG), John S. Hendricks (JSH), H. Grady Hughes (HGH), Julian Lebenhaft (JL), Robert C. Little (RCL), Stepan G. Mashnik (SGM), Douglas R. Mayo (DRM), Gregg W. McKinney (GWM), Eric J. Pitcher (EJP), Richard E. Prael (REP), Teresa L. Roberts (TLR), Arnold J. Sierk (AJS), Edward C. Snow (ECS), Avneet Sood (AS), Martyn T. Swinhoe (MTS), Stephen J. Tobin (SJT), Laurie S. Waters (LSW), Christopher J. Werner (CJW), and Morgan C. White (MCW).

MCNPX 2.5.d (August 2003)

- INCL4/ABLA physics models (JCD/JSH);
- lattice tally speedup (GWM);
- auxiliary input files: READ (JSH);
- geometry plot of WWG superimposed mesh (JSH);
- pulse-height light tally with anticoincidence: FT8 PHL (GWM);
- coincidence capture tally and PTRAC file: FT8 CAP (MTS/SJT/DRM/JSH);
- residual nuclei tally: FT8 RES (JSH); and
- inline generation of double differential cross sections and residuals (JSH).

MCNPX 2.5.c (April 2003)

- message passing interface (MPI) multiprocessing (JL/GWM);
- i,j,k lattice indexing in geometry plots (JSH);
- enable of WWG in physics model region (FXG/ JSH);
- enablement of exponential transform in physics model region (FXG/JSH);
- extension of neutron model physics below 20 MeV (JSH);
- ³He coincidence detector modeling (HGH/JSH); and
- F90 autoconfiguration (TLR).

MCNPX 2.5.b (November 2002)

- CEM2k physics (SGM/AJS/FXG);
- mix and match (JSH);
- positron sources (HGH); and
- spontaneous fission (JSH).

MCNPX 2.4.0 (August 2002)

- F90 modularity and dynamic memory allocation (GWM);
- distributed memory multiprocessing for the entire energy range of all particles (GWM);
- repeated structures source-path improvement (LLC/JSH);
- default dose functions (LSW/JSH);
- light-ion recoil (JSH);
- enhanced color geometry plots (GWM/JSH);
- photonuclear cross-section plots (JSH);
- proton cross-section plots (JSH);
- proton reaction multipliers with FM cards (JSH);
- photonuclear reaction multipliers with FM cards (JSH/GWM);
- some speedups (GWM/JSH);
- logarithmic interpolation on input cards (JSH);
- cosine bins that may be specified in degrees (JSH);
- cosine bins that may be specified for F2 flux tallies (JSH);
- source particles that may be specified by descriptors (JSH); and
- pause command for tally and cross-section plots (JSH).

MCNPX 2.3.0 and previous MCNPX versions (1995 to 2001)

- physics for 34 particle types (HGH);
- high-energy physics above the tabular data range (REP);
- photonuclear physics (MCW);
- neutron, proton, and photonuclear 150-MeV libraries and use (RCL);
- mesh tallies (tallies in a superimposed mesh) (LSW/ECS);
- radiography tallies (JSH/ECS);
- secondary-particle production biasing (ECS); and
- autoconfiguration build system for compilation (TLR/HWE).

MCNP4C3, MCNP4C2, and MCNP4C features added after MCNP4B (1997–2001)

- PC enhancements: Linux and Windows capable (LLC/GWM);
- easier geometry specification with macrobodies (LLC);
- interactive geometry plotting (JSH);
- improved variance reduction with the superimposed mesh WWG (TME/JAF/JSH);
- superimposed mesh plotting (JSH);
- delayed neutrons (CJW);
- unresolved resonance range probability tables (LLC/RCL);
- perturbations for material-dependent tallies (GWM/LLC/JSH);
- ENDF/B-VI extensions (MCW);
- electron physics enhancements (upgrade to ITS3.0)* (KJA/HGH);
- weight-window enhancements (JSH/JAF); and
- distributed memory multiprocessing (GWM).

10.0. FUTURE WORK

- CINDER90 capabilities:
 - delayed neutrons physics models;
 - delayed gamma physics models; and
 - transmutation.
- improved high-energy physics with the LAQGSM model;
- heavy-ion tracking and interactions;
- criticality:
 - externally driven sources and
 - improved stability of eigenfunctions.
- plotting of physics model total and absorption cross sections;
- forced collisions for neutral particles extended to physics models;
- secondary particle angle biasing for isotropic distributions;
- neutral particle perturbation techniques extended to physics model region;
- heavy-ion tracking and interactions;
- interactive tally and cross-section plotting;

* J. A. Halbleib, R. P. Kensek, T. A. Mehlhorn, G. D. Valdez, S. M. Seltzer, M. J. Berger, "ITS Version 3.0: The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport Codes," Sandia National Laboratories report SAND91-1634 (March 1992).

- detectors and DXTRAN for all neutral particles at all energy ranges;
- a capability to continue runs that write HTAPE files;
- integration of HTAPE tallies directly into MCNPX;
- CAD link; and
- magnetic field tracking.

11.0. BIBLIOGRAPHY

11.1. Code Manuals

Laurie S. Waters, ed., “MCNPX User’s Manual, Version 2.4.0,” Los Alamos National Laboratory report LA-CP-02-408 (September 2002).

Laurie S. Waters, ed., “MCNPX User’s Manual, Version 2.3.0,” Los Alamos National Laboratory report LA-UR-02-2607 (April 2002).

J. F. Briesmeister, ed., “MCNP—A General Monte Carlo N-Particle Transport Code—Version 4C,” Los Alamos National Laboratory report LA-13709-M (April 2000).

Laurie S. Waters, ed., “MCNPX User’s Manual—Version 2.1.5,” Los Alamos National Laboratory report LA-UR-99-6058 (November 14, 1999).

J. F. Briesmeister, ed., “MCNP—A General Monte Carlo N-Particle Transport Code—Version 4B,” Los Alamos National Laboratory report LA-12625-M (March 1997).

J. A. Halbleib, R. P. Kensek, T. A. Mehlhorn, G. D. Valdez, S. M. Seltzer, and M. J. Berger, “ITS Version 3.0: The Integrated TIGER Series of Coupled Electron/Photon Monte Carlo Transport Codes,” Sandia National Laboratories report SAND91-1634 (March 1992).

11.2. Code Version Release Announcements

John S. Hendricks et al., “MCNPX, Version 2.5.F,” Los Alamos National Laboratory report, LA-UR-05-0891 (February 2005).

John S. Hendricks et al., “MCNPX, Version 2.5.E,” Los Alamos National Laboratory report, LA-UR-04-0569 (February 2004).

John S. Hendricks et al., “MCNPX, Version 2.5.D,” Los Alamos National Laboratory report, LA-UR-03-5916 (August 2003).

John S. Hendricks et al., “MCNPX, Version 2.5.C,” Los Alamos National Laboratory report LA-UR-03-2202 (April 2002).

John S. Hendricks and the MCNPX Team, “MCNPX, Version 2.5.B,” Los Alamos National Laboratory report LA-UR-02-7086 (November 2002).

MCNPX Team, "MCNPX, Version 2.4.0," Los Alamos National Laboratory report LA-UR-02-5253 (August 2002).

John S. Hendricks, "MCNP4C3," Los Alamos National Laboratory report LA-UR-01-2244 (April 13, 2001).

John S. Hendricks, "MCNP4C2," Los Alamos National Laboratory report LA-UR-01-858 (January 30, 2001).

John S. Hendricks, "MCNP4C," Los Alamos National Laboratory memorandum X-5:JSH-2000-30 (February 29, 2000).

John S. Hendricks, "MCNP4B," Los Alamos National Laboratory memorandum XTM:JSH-97-13 (January 31, 1997).

11.3. Reports

John S. Hendricks, "MCNPX Model/Table Comparison," Los Alamos National Laboratory report LA-14030 (March 2003).

11.4. Papers

J. S. Hendricks, G. W. McKinney, J. W. Durkee, M. R. James, D. B. Pelowitz, and H. R. Trelue, "The MCNPX Radiation Transport Code," Los Alamos National Laboratory report LA-UR-05-0683, submitted to M&C 2005, the International Topical Meeting on Mathematics and Computation, Avignon, France (September 12–15, 2005).

John S. Hendricks and Jane M. Burward-Hoy, "Monte Carlo Radiation Detector Modeling in Space Systems," Los Alamos National Laboratory report LA-UR-05-1841, submitted to Space Nuclear Conference (SNC '05), San Diego, California (June 6–9, 2005).

M. James, J. Durkee, J. Hendricks, G. McKinney, D. Pelowitz, and F. Gallmeier, "Physics Improvements in MCNPX 2.5.0," International Collaboration on Advanced Neutron Sources, ICANS XVII, Santa Fe, New Mexico (April 25–29, 2005).

G. McKinney, J. Durkee, J. Hendricks, M. James, D. Pelowitz, and F. Gallmeier, "New MCNPX 2.5.0 Features," International Collaboration on Advanced Neutron Sources, ICANS XVII, Santa Fe, New Mexico (April 25–29, 2005).

John S. Hendricks, "Monte Carlo Sampling of Fission Multiplicity," Los Alamos National Laboratory report LA-UR-04-6967, submitted to Monte Carlo 2005, Chattanooga, Tennessee (April 17–21, 2005).

John S. Hendricks and Gregg W. McKinney, "Pulse-Height Tallies with Variance Reduction," Los Alamos National Laboratory report LA-UR-04-8431, submitted to Monte Carlo 2005, Chattanooga, Tennessee (April 17–21, 2005).

Joshua P. Finch, John S. Hendricks, Chan K. Choi, “Vacation Matrix Method for Correct Source Distribution in Monte Carlo Criticality Calculations,” Los Alamos National Laboratory report LA-UR-04-8595, submitted to Monte Carlo 2005, Chattanooga, Tennessee (April 17–21, 2005).

G. W. McKinney, J. W. Durkee, J. S. Hendricks, M. R. James, D. B. Pelowitz, and L. S. Waters, “MCNPX 2.5.0—New Features Demonstrated,” Los Alamos National Laboratory report LA-UR-04-8695, submitted to Monte Carlo 2005, Chattanooga, Tennessee (April 17–21, 2005).

Martyn T. Swinhoe, John S. Hendricks, and Douglas R. Mayo, “MCNPX for Neutron Multiplicity Detector Simulation,” Los Alamos National Laboratory report LA-UR-04-8025, submitted to European SAFeguards Research and Development Association (ESARDA) Symposium on Safeguards and Nuclear Material Management, London, United Kingdom (June 2005).

J. S. Hendricks, G. W. McKinney, L. S. Waters, and F. X. Gallmeier, “New MCNPX Capabilities,” Los Alamos National Laboratory report LA-UR-04-0193, *Transactions of the American Nuclear Society*, Pittsburgh, PA **90**, 475 (June 13–17, 2004).

J. S. Hendricks, J. P. Finch, and C. Choi, “Calculation of Eigenfunction Fluxes in Nuclear Systems,” Los Alamos National Laboratory report LA-UR-03-2917, American Nuclear Society Topical Meeting, Radiation Protection and Shielding Division, ICRS-10/RPS 2004, Madiera, Portugal, published by Instituto Tecnológico e Nuclear, Sacavem, Portugal (May 10–14, 2004).

G. W. McKinney, J. S. Hendricks, H. R. Trellue, and L. S. Waters, “Eigenfunction Convergence and Transmutation Enhancements in MCNPX,” Los Alamos National Laboratory report LA-UR-03-7714, submitted to PHYSOR-2004, American Nuclear Society Topical Meeting, Reactor Physics Division, Chicago, Illinois (April 25–29, 2004).

J. S. Hendricks, M. T. Swinhoe, S. J. Tobin, W. H. Geist, and D. R. Mayo, “Neutron Multiplicity Counting for Nuclear Safeguards with MCNPX,” Los Alamos National Laboratory report LA-UR-03-0456 (2003).

J. S. Hendricks, G. W. McKinney, L. S. Waters, and Franz X. Gallmeier, “MCNPX Advances for Accelerator Applications,” *Sixth International Meeting on the Nuclear Applications of Accelerator Technology (AccApp’03)*, American Nuclear Society Embedded Topical Meeting, San Diego, California (June 1–5, 2003), Los Alamos National Laboratory report LA-UR-03-0075.

John S. Hendricks, Gregg W. McKinney, and Franz G. Gallmeier, “Mix and Match with MCNPX,” *Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew*, Gatlinburg, Tennessee, on CD-ROM (American Nuclear Society, LaGrange Park, Illinois), ANS order no. 700300, ISBN: 0-89448-674-8 (April 6–11, 2003), Los Alamos National Laboratory report LA-UR-02-6415 (2002).

J. S. Hendricks, G. W. McKinney, L. S. Waters, H. G. Hughes, and E. C. Snow, “New MCNPX Developments,” Los Alamos National Laboratory report LA-UR-02-2181 (April 2002).

Stepan G. Mashnik and Arnold J. Sierk, "Recent Developments of the Cascade-Exciton Model of Nuclear Reactions," International Conference on Nuclear Data for Science and Technology, October 7–12, 2001, Tsukuba, Japan. *Nuclear Science and Technology, Supplement 2*, 720–725 (2002): <http://lib-www.lanl.gov/la-pubs/00818526.pdf>.

E. C. Selcow, G. W. McKinney, T. E. Booth, J. F. Briesmeister, L. J. Cox, R. A. Forster, J. S. Hendricks, R. D. Mosteller, R. E. Prael, A. Sood, and S. W. White, "MCNP Capabilities at the Dawn of the 21st Century: Neutron-Gamma Applications," Los Alamos National Laboratory report LA-UR-00-5017 (2000).

J. S. Hendricks, K. J. Adams, T. E. Booth, J. F. Briesmeister, L. L. Carter, L. J. Cox, J. A. Favorite, R. A. Forster, G. W. McKinney, and R. E. Prael, "Present and Future Capabilities of MCNP," *Applied Radiation and Isotopes* **53**:4-5, 857–861 (2000).

J. S. Hendricks, "Advances in MCNP4C," Los Alamos National Laboratory report LA-UR-00-2643 (2000).

G. W. McKinney, T. E. Booth, J. F. Briesmeister, L. J. Cox, R. A. Forster, J. S. Hendricks, R. D. Mosteller, R. E. Prael, and A. Sood, "MCNP Applications for the 21st Century," in "Proceedings of the 4th International Conference on Supercomputing in Nuclear Applications," Tokyo, Japan (September 4–7, 2000).

J. S. Hendricks, G. W. McKinney, and L. J. Cox, "Monte Carlo Advances for the Eolus ASCI Project," PHYSOR2000 International Topical Meeting on Advances in Reactor Physics and Mathematics and Computation, Pittsburgh, Pennsylvania, May 7–11, 2000.

K. J. Adams, T. E. Booth, J. F. Briesmeister, L. L. Carter, J. D. Court, L. J. Cox, J. A. Favorite, R. A. Forster, J. S. Hendricks, G. W. McKinney, and R. E. Prael, "Present and Future Capabilities of MCNP," in "Fourth Topical Meeting on Industrial Radiation and Radioisotope Measurement Applications (IRRMA 99)," Raleigh, North Carolina (October 3–7, 1999), p. 38.

H. G. Hughes, K. J. Adams, M. B. Chadwick, J. C. Comly, L. J. Cox, H. W. Egdorf, S. C. Frankle, J. S. Hendricks, R. C. Little, R. E. MacFarlane, S. G. Mashnik, R. E. Prael, A. J. Sierk, L. S. Waters, M. C. White, P. G. Young, Jr., F. Gallmeier, and E. C. Snow, "MCNPX for Neutron-Proton Transport," in "Proceedings of Mathematics and Computation, Reactor Physics, and Environmental Analysis in Nuclear Applications," Madrid, Spain, Vol. 2, pp. 939–948 (September 1999).

Stepan G. Mashnik and Arnold J. Sierk, "Improved Cascade Exciton Model of Nuclear Reactions," in "Proceedings of the Fourth Workshop on Simulating Accelerator Radiation Environments (SARE4)," Knoxville, Tennessee, September 14–16, 1998, T. A. Gabriel, Ed. (Oak Ridge National Laboratory, Oak Ridge, Tennessee, 1999), pp. 29–51.

H. G. Hughes, K. J. Adams, M. B. Chadwick, J. C. Comly, L. J. Cox, H. W. Egdorf, S. C. Frankle, F. X. Gallmeier, J. S. Hendricks, R. C. Little, R. E. MacFarlane, R. E. Prael, E. C.

Snow, L. S. Waters, M. C. White, and P. G. Young, Jr., “Recent Developments in MCNPX,” in “Proceedings of the Second International Topical Meeting on Nuclear Applications of Accelerator Technology,” Gatlinburg, Tennessee (September 20–23, 1998), p. 281.

12.0. ACKNOWLEDGMENTS

The authors wish to thank Lisa Rothrock and Tamara Hallman of group IM-1 for their editing of this document.