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MCNPX, VERSION 2.5.d

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ABSTRACT

MCNPX is a Fortran90 Monte Carlo radiation transport computer code that transports all particles at all energies. It is a superset of MCNP4C3 and has many capabilities beyond MCNP4C3. These capabilities are summarized in this report, along with the MCNPX quality guarantee and code availability. In addition, the new capabilities of the latest version, MCNPX 2.5.d, are described.

1.0. INTRODUCTION

MCNPX is a Fortran90 (F90) Monte Carlo radiation transport computer code that transports all particles at all energies. MCNPX stands for MCNP eXtended. It is a superset of MCNP4C3 and has many capabilities beyond MCNP4C3. MCNPX is a production computer code for modeling the interaction of radiation with matter, and its quality is guaranteed; it can be used with confidence. MCNPX is available from the Radiation Safety Information and Computational Center (RSICC) and the Office of Economic Community Development (OECD)/Nuclear Energy Agency (NEA). For approved users, beta test program versions may be downloaded from the MCNPX website at http://mcnpx.lanl.gov.

1.1. New MCNPX 2.5.d Capabilities

MCNPX 2.5.d offers many new capabilities. Where applicable, the initials of the principal developers are shown in parentheses.* The complete summary of MCNPX capabilities beyond MCNPX 2.3.0 and MCNP4C is provided in the MCNPX features list available on the MCNPX website at http://mcnpx.lanl.gov.

- INCL4/ABLA physics models (JCD/JSH);
- lattice tally speedup (GWM);
- multiple particles on SDEF card (JSH);
- SDEF cylindrical sources (JSH);
- auxiliary input files: READ card (JSH);
- geometry plot of weight-window-generator 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);
- inline generation of double differential cross sections and residuals (JSH); and
- corrections/enhancements/extensions.

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In addition, the MCNPX test set has been upgraded completely in MCNPX 2.5.d (JPF) to include the MCNP5 test set (slightly modified) as a subset and to test many recent MCNPX capabilities.

1.2. Guarantee

MCNPX is guaranteed. We are so confident of the quality of MCNPX that we will pay $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 given for problems carrying over from older code versions; very few errors have been found in the new MCNPX versions. A listing of winners is available at http://mcnpx.lanl.gov. MCNPX bugs are described in the release notes for each MCNPX version.

1.3. Availability

MCNPX 2.4.0 is available from the RSICC in Oak Ridge, Tennessee, USA, at http://www-rsicc.ornl.gov. MCNPX 2.4.0 is also available from the OECD NEA Data Bank in Paris, France, at http://www.nea.fr.

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 1000 MCNPX beta testers worldwide. MCNPX 2.5.d is available to beta testers on the MCNPX website at http://mcnpx.lanl.gov. To apply for a beta test password and to have access to the latest MCNPX versions, contact Laurie Waters at lsw@lanl.gov.

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

2.0. DESCRIPTION OF NEW MCNPX 2.5.d FEATURES

2.1. INCL4/ABLA (Cugnon/Schmidt) Physics Models

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

LCA(9)	= 0	Bertini model if LCA(3) = 1
		Bertini/ISABEL model if LCA(3) = 2
	= 1	CEM2k model (LCA(3) ignored)

[*] Cash Award Fine Print: This offer is subject to cancellation or modification without notice. A bug is defined as an error we chose to correct in the source code. 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 have the most error-free and robust Monte Carlo radiation transport capabilities, and we back them with a cash guarantee.

	= 2	INCL4 model (LCA(3) = 0 by INCL default)
LEA(7)	= 0	Dresner evaporation
	= 2	ABLA evaporation
LCC(1)	= sti	= 1, stopping time parameter in INCL

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) iexisa	LCA(9) imodec	LEA(7) ievap
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

2.1.1. Description of INCL4

The INCL4 model is based largely on the work of Joseph Cugnon at the University of Liege in Liege, Belgium. It generally is coupled with the ABLA evaporation model that was developed principally by Karl-Heinz Schmidt at Gesellschaft für Schwerion-enforschung, mbH, Darmstadt, Germany. 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. There are only two free parameters in INCL4: the potential depth V_0 (default = 45 MeV) and the overall factor f_{stop} (default = 1.0), which governs the stopping time and is STI on the LCC card.

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

2.2. Lattice Tally Speedup

Input files with large lattice tallies now run 10–1000 times faster if the following apply:

- The lattice is specified fully on the cell fill card, e.g., FILL –50:50 –50:50 –50:50.

- The tallies refer to no more than one cell at each level, except for the lattice cell, which can be a range of values:
  F4:p (1 < 2 < 3[–50:50 –50:50 –50:50] < 4).

  The following will not work:
  F4:p (1 < 2 < 3[–50:50 –50:50 –50:50] < 4 5)

  because two cells, 4 and 5, were specified at the top level.

The reader is invited to try a lattice tally with MCNPX 2.5.d and a version without this new capability to see the differences in the histories run per minute and in the Figure of Merit.

2.2.1. Example

The following simple input file runs 70 times faster with MCNPX 2.5.d than with MCNPX 2.5.c and previous MCNP 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)
```

2.2.2. Notes

- Larger lattices and nested lattices offer even more dramatic speedups but take longer to demonstrate than the simple example shown in Section 2.2.1.

- The fast lattice capability requires slight additional time to set up the problem before histories are run. A problem that takes 10 minutes to set up and 100 hours to run histories now may take 15 minutes to set up and 1 hour to run histories.

2.3. Multiple Particles on SDEF Card

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

2.3.1. 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).

2.3.2. 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 2.3.1 exactly.

2.3.3. 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 .

2.3.4. Tally and Summary Table Normalizations

Tallies are normalized by dividing the total source weight by the number of source histories. Note that 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 2.3.1,

```
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 protons that are produced is 0.6667. From the SB1 card, the total number of neutron tracks is 0.6667 × NPS for neutrons and 0.3333 × 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, 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 by fission neutrons (plus other source particle) 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.

2.4. SDEF Cylindrical Sources

Cylindrical surface sources now may be specified on the SDEF card. Furthermore, particle directions distributed 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.

2.4.1. 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 .

2.4.2. 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 now may be specified on a cylindrical surface, and the default VEC is the surface normal;
    - DIR now may be specified without VEC (so that VEC defaults to the surface normal) for spheres and cylinders; and
    - the outward normal to cylindrical surfaces now is generated whenever DIR is specified and VEC is not.

2.5. Auxiliary Input File and Encryption

The new 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.

2.5.1. 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.

2.5.2. 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 .

Whereas the default of the READ card is ECHO, the echoing 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.

2.5.3. 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.

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

MCNPX can plot the weight-window-generator (WWG) superimposed mesh specified on the MESH card in an input file. The following options are now 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

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 0–5, as determined by the options list above.

The ability to plot the WWG mesh, options *mesh = 4* and *mesh = 5*, is new in MCNPX 2.5.d.

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 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 weight-window generator 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).

2.6.1. 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. 1)
	Zoom 10	to get 10x magnification (click twice)
	Origin	click in the center of material to center picture
	ZX	to get py = 5 view (radial view, Fig. 2)

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

A new FT option is available for pulse-height (F8) tallies, which allows the F8 tally to 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} ... ,

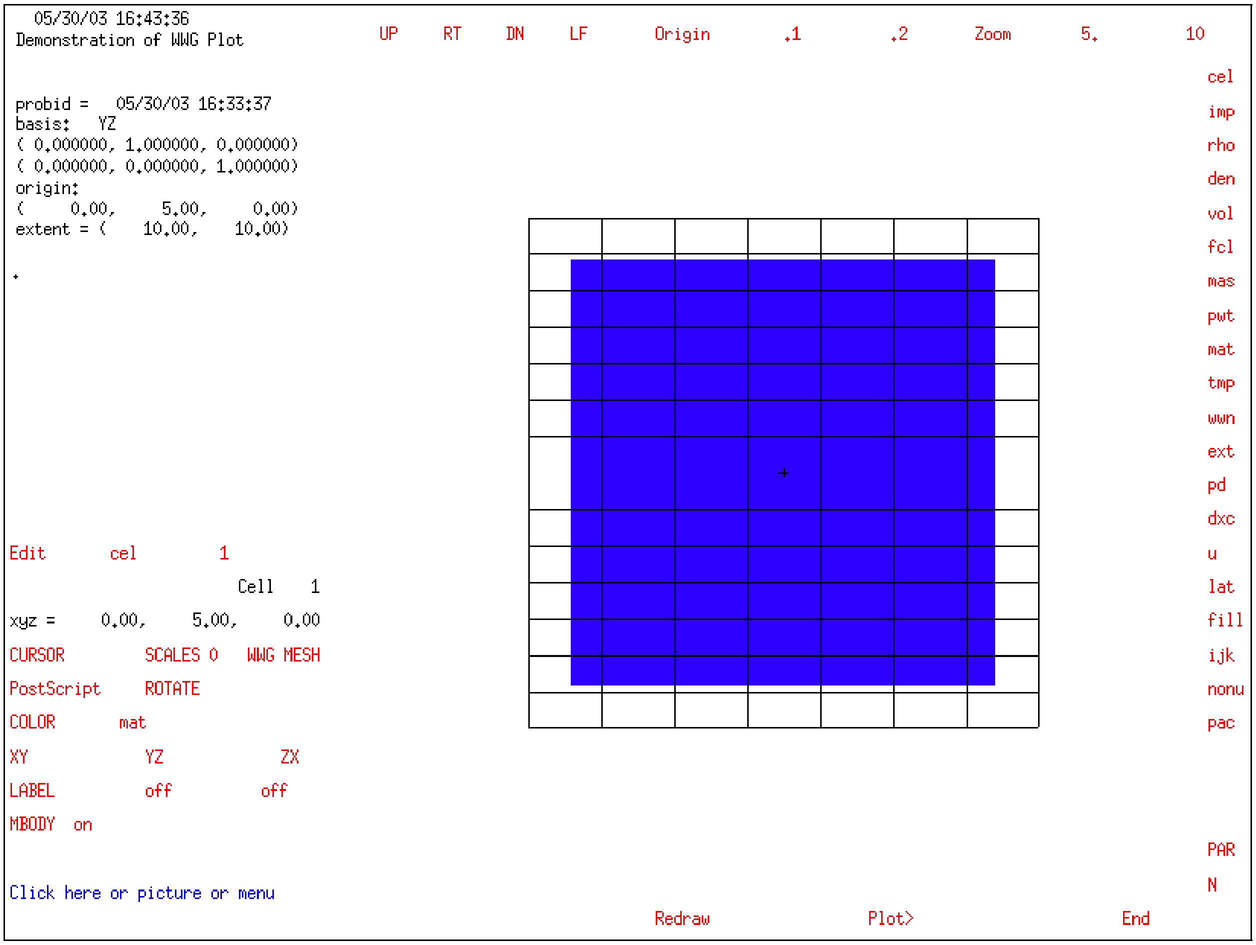

Fig. 1. WWG mesh plot, axial view.

where

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

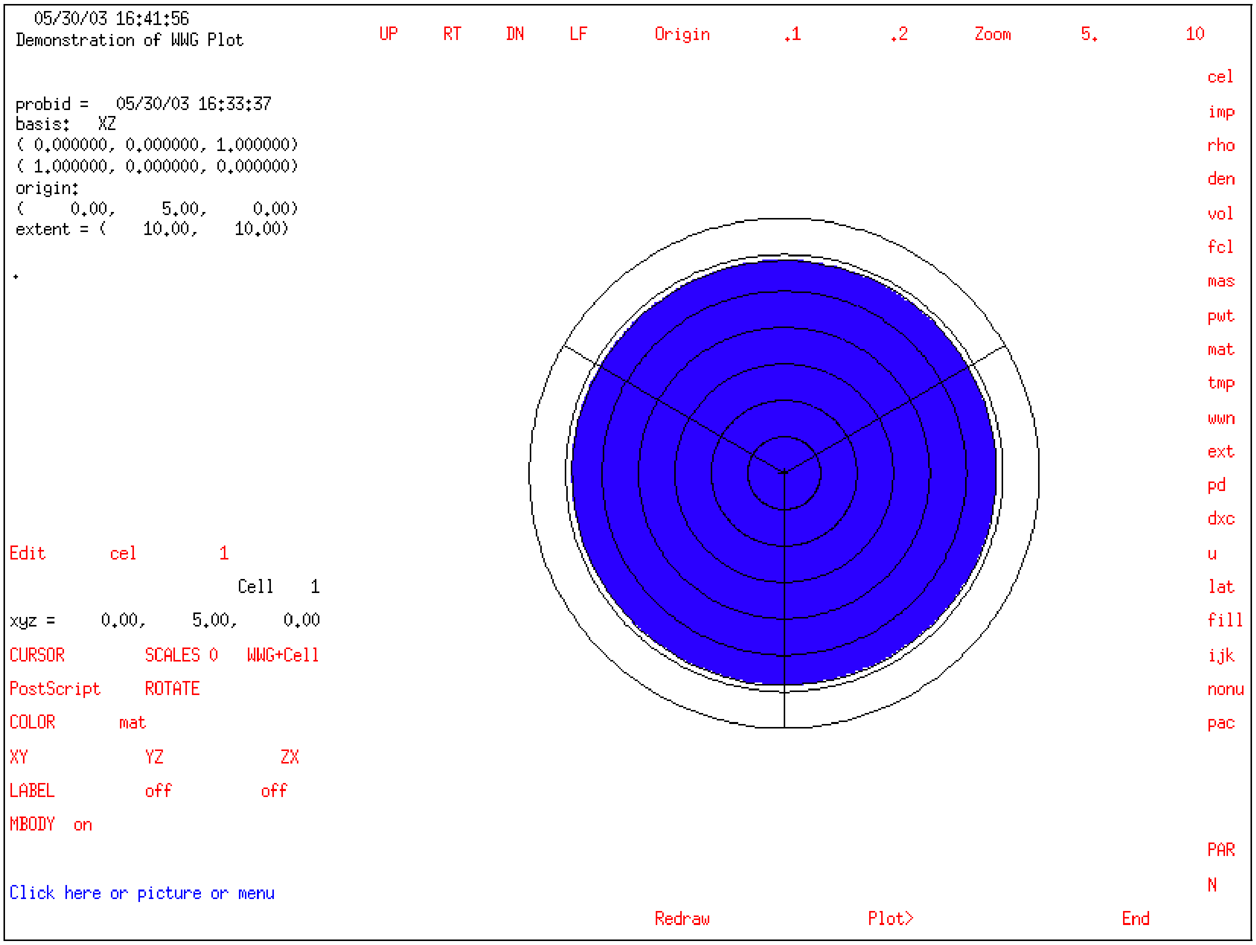

Fig. 2. WWG plot, radial view.

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.

2.7.1. 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 because the PHL tally renormalizes 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 (DL) 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 is done only at the end of the particle history to determine the light output value used in the pulse-height tally.

In Case 1, the electron light output from only one region (cell 5) is used to subdivide the pulse-height tally. 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 pulse-height tally. 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. Note that 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 2 6 1 6 2 0
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 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.

2.7.2. Coincidence Detector Capture Tally and PTRAC File: FT8 CAP

The ^{3}He coincidence detector capability of previous MCNPX versions has been upgraded significantly to a more general capture tally. An F8 tally is used, rather than a COINC card, to take advantage of many tally features, particularly the following:

- capture tallies can be made by any nuclide or combination of nuclides, not just ^{3}He;
- multiple capture tallies may be used in a single run, not just one COINC card;
- tally cells may be combined, grouped or totaled;
- time bins are enabled;
- tally plots are enabled;
- user-supplied TALLYX subroutines are available;
- tally fluctuation charts are enabled; and
- tally statistical analysis is available.

In addition, captures may be written to an auxiliary output file, PTRAC. Section 2.7.6 describes the PTRAC capture file.

2.7.3. Comparison to the MCNPX 2.5.c COINC Card Capability

In MCNPX 2.5.c and earlier, the ^{3}He coincidence detector model input was

```
COINC 2 5 6 7   .
```

This input would tally the capture multiplicity and moments of ^{3}He in cells 2, 5, 6, 7.

The new interface is

```
F8:n 2 5 6 7
FT8     CAP    2003   .
```

The F8 tally results in the identical tally and printout for ^{3}He coincidence capture, as was provided by the COINC card capability. Note that the COINC input card is no longer recognized.

2.7.4. Example of the New FT8 CAP Capability

An example of the new FT8 CAP capability is

```
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; the combination of 5 and 6; and in the total over cells 2, 5, 6, 7. The captures by either ^{6}Li or ^{10}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 nanoseconds to 1 second.

Capture multiplicities and moments require analog capture. The presence of "cap" on the FT8 card forces CUT:N 2J 0 0, which specifies neutron analog capture. 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.

Print Table 118 lists the multiplicities and moments for each bin of the capture tally as follows.

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

 cell:    22

 neutron captures on   3006   5010   2003
                         captures          captures          multiplicity fractions
             histories  by number         by weight        by number         by weight        error

 captures =  0     586          0      0.00000E+00      5.86000E-01      2.86133E-01      0.0266
 captures =  1     255        255      1.24512E-01      2.55000E-01      1.24512E-01      0.0541
 captures =  2      53        106      5.17578E-02      5.30000E-02      2.58789E-02      0.1337
 captures =  3      15         45      2.19727E-02      1.50000E-02      7.32422E-03      0.2563
 captures =  4       5         20      9.76562E-03      5.00000E-03      2.44141E-03      0.4461
 captures =  5       2         10      4.88281E-03      2.00000E-03      9.76562E-04      0.7064

    total          916        436      2.12891E-01      1.00000E+00      1.00000E+00      0.0534

      factorial moments             by number              by weight

             cap               4.36000E-01 0.0534      2.12891E-01 0.0556
        cap(cap-1)/2!          1.48000E-01 0.1579      7.22656E-02 0.1587
     cap(cap-1)(cap-2)/3!      5.50000E-02 0.3107      2.68555E-02 0.3111
  cap(cap-1) .... (cap-3)/4!   1.50000E-02 0.4934      7.32422E-03 0.4936
  cap(cap-1) .... (cap-4)/5!   2.00000E-03 0.7064      9.76562E-04 0.7066


 ascii   file ptrak   written with    2106 events from     916 histories.
```

For capture tallies on the single nuclides ^{3}He, ^{6}Li, or ^{10}B, the nuclide name 3he, 6li, or 10b is listed instead of "cap."

2.7.5. Possible Future Extensions of FT8 CAP Option

The coincidence counter capture tally model lacks many standard tally features to make the algorithm faster. If desired, 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.

2.7.6. PTRAC Capture File

The 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) is very different from the usual PTRAC data. 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 = particle history number,
time = time from source event to analog capture in any FT8 cap tally,
cell = cell in which analog capture occurred, and
source = 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, there is no history 2.

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.

2.7.7. 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.*

2.7.8. Possible Future Extensions of the PTRAC Capture Option

Many standard PTRAC capabilities are missing from the PTRAC capture tally output file capability. These could be added, if desired, 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.

2.8. Residual Nuclei Tally: FT8 RES

A new special tally treatment (FT card) option (RES) is now available to tally residual nuclei in the physics model region.

The form of the FT card is

FT8 RES

or

FT8 RES Z_1 Z_2 .

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 utilizing 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 Z_1 and Z_2, which correspond to a range of possible Z values. If Z_1 and Z_2 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. If LCA(8) = –2, then the residuals from a single inelastic reaction may be tallied (see Section 2.9).

2.9. Inline Generation of Double Differential Cross Sections and Residuals

A new 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. The following input files model a 1.2-GeV proton source having a single collision with ^{208}Pb.

```
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
print
prdmp 2j -1 2
nps 10000
f8:h 1
ft8 res 1 99
fq8 u e
fq1 e c
*c1 167.5 9i 17.5 0 T
e1 1 50log 1300 T
fc1  *** neutron angle spectra tally ***
f1:n  1
ft1  frv 0 0 1
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 the following execute line command:

MCNPX Z ,

where the command file, COM91, is

```
rmctal=mctl91
file all loglog xlim 1 1300 ylim 1e-6 1 fix c 13
pause
fix c 13 cop fix c 1 cop fix c 6 cop fix c 12
pause
tally 8 free u xlim 80185 80205 ylim .0001 .01
pause
xlim 81189 81208
pause
xlim 82188 82208
pause
xlim 82188 82208 ylim .0001 1
pause
xlim 83190 83215 ylim 1e-4 1e-2
pause
end
```

In Fig. 3, the first line (solid black) is the energy spectrum over all angles, the second (blue dashed) is the 180^o output, the third (red dotted) is the 90^o output, and the fourth (green broken) is the 0^o output.

The residuals for ${}_{81}Tl$ isotopes 189–201 are plotted in Fig. 4.

When NOACT = –2 on the LCA card, then the source particle immediately collides in the source material. All subsequent daughter particles then are transported without further collision, as if in a vacuum. A properly specified F1 surface current tally then provides the double differential cross section, namely the energies and angles of the daughter particles. An F8 tally with an FT8 RES special tally treatment can be used to provide the residuals, namely the distribution of nuclides resulting from the collision.

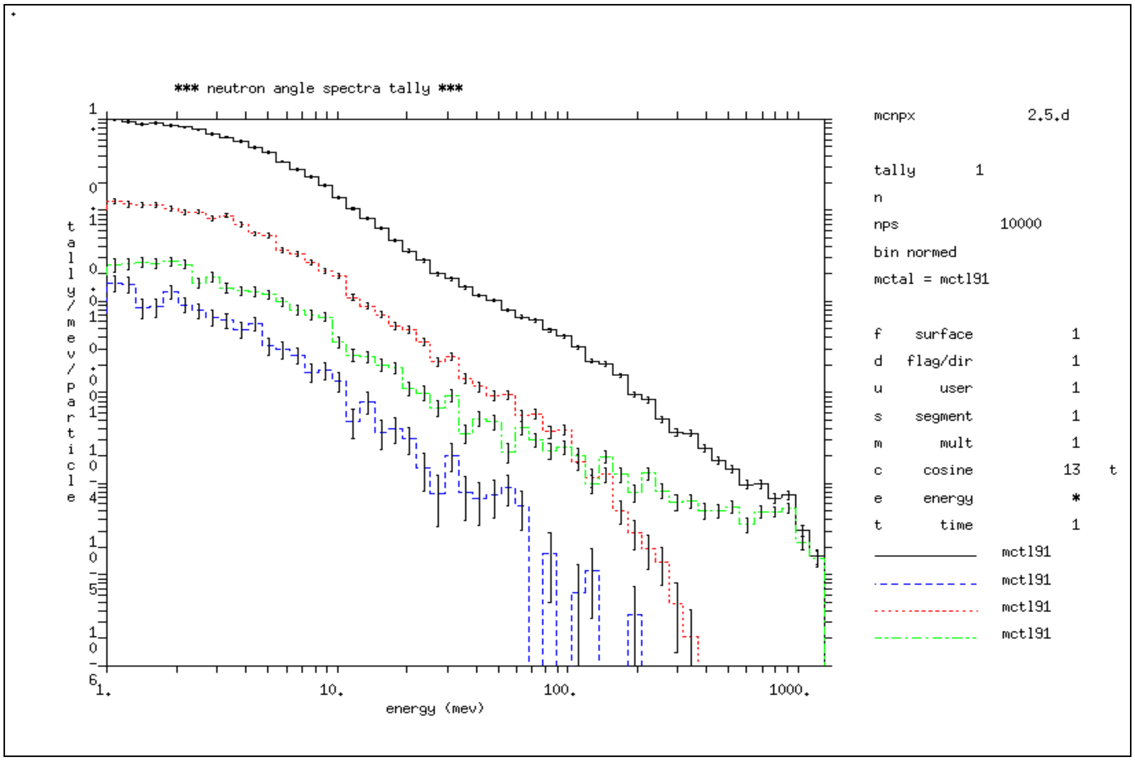

Fig. 3. Differential cross sections at all angles, 180°, 90°, and 0° for 1.3-GeV protons on $^{208}_{82}$Pb.

3.0. MCNPX 2.5.d FEATURE EXTENSIONS AND ENHANCEMENTS

Several MCNPX features have been extended and have changes or additions to the user interface.

3.1. Spontaneous Fission Normalization

The spontaneous fission source now can be specified in one 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 fission neutrons).

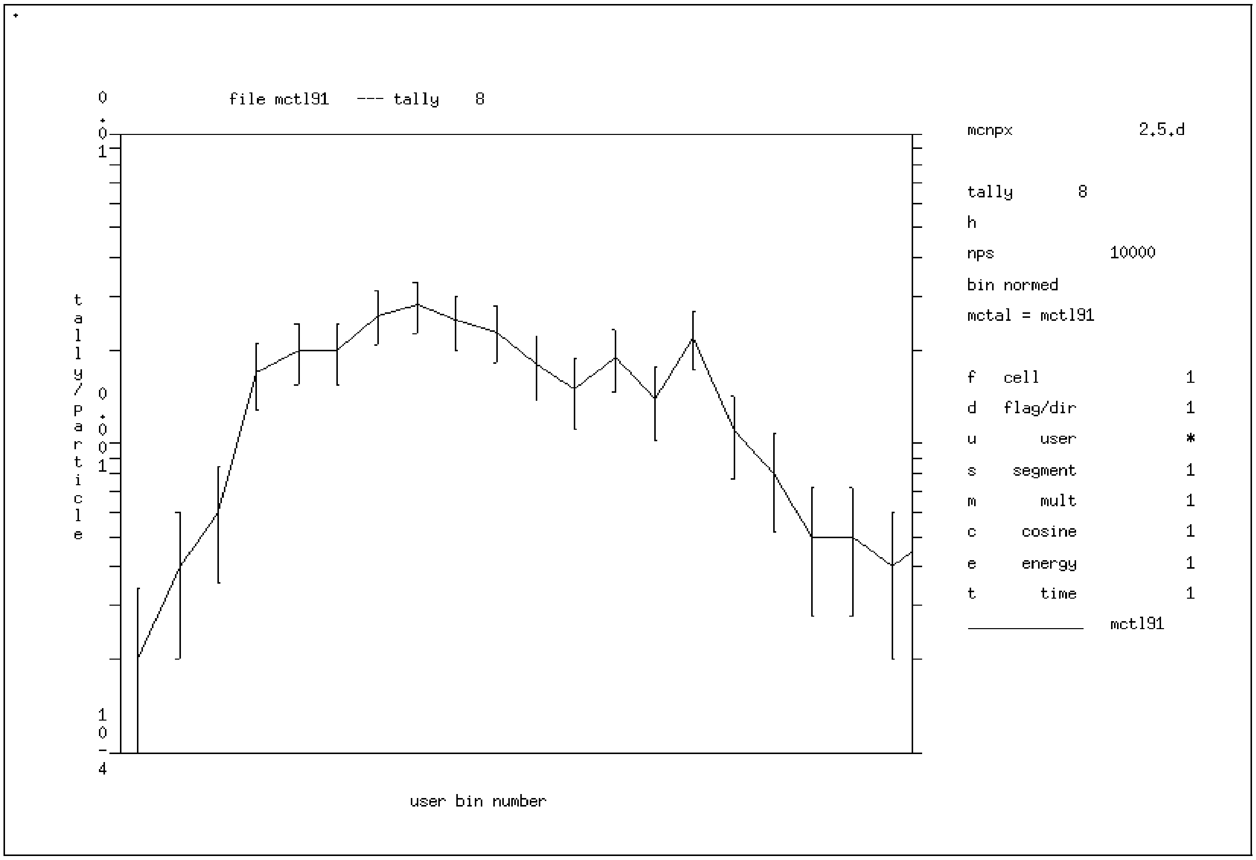

Fig. 4. Residuals for $_{81}$T1 isotopes 189–201 from 1.3-GeV protons on $^{208}_{82}$Pb.

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 = ν·N,
summary table source weight = W,
summary tables and tallies are normalized by ν·N.

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

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

Additionally, the ^{252}Cf spontaneous fission Watt spectrum source energy parameters have been changed from the MCNP5 values to a = 1.18 and b = 1.03419 for better experimental agreement.

3.2. MCNP5 Capabilities

Many extensions have been made to maintain compatibility with MCNP5.*
Often these changes are small because many new MCNP5 features already were included in MCNPX.

- Radiography tallies: translate new MCNP5 FIP, FIR, and FIC radiography input cards as MCNPX radiography tallies PI, TIR, and TIC.
- Increase allowable ESPLT entries from 10 to 20.

Other MCNP5 capabilities not already incorporated into MCNPX likely will be added as requested by MCNPX users.

3.3. HISTP Card Options

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

HISTP –lhist icl_1 icl_2 icl_3 .

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 continues 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.

icl_1, icl_2, … 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*.

* 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).

3.3.1. Examples

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

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.

3.4. Additional Enhancements

The following enhancements were made to MCNPX 2.5.c in addition to the major new capabilities explained in Section 2.0. These enhancements do not affect the user interface.

3.4.1. +F8 Charged-Particle Deposition

The net charged particle energy deposition +F8 tally has been expanded to protons and charged particles other than electrons.

3.4.2. Locating Cross Sections in Continue Runs

Previously, MCNPX did not remember the DATAPATH in continue runs. The location of the model physics data tables, barpol.dat, bertin, phtlib, and optional CEM gdr.dat and INCL .data and .tab files must be available to a continue-run problem because these files are reread during continue runs. Not remembering the DATAPATH in continue runs was no problem in most cases where the DATAPATH is set (Unix systems) or else these data are in the default MCNPX directories or the directory where the problem is being run. However, if the DATAPATH is set some other way, such as in the XSDIR file or in the INP message block, then MCNPX cannot find the data. The only recourses were to move the libraries to the local space or to specify the DATAPATH in the continue-run INP file. MCNPX 2.5.d "remembers" the DATAPATH where the data were located in the initial run, thus solving the annoying problem of not finding the data libraries in some continue runs (GWM/JSH).

3.4.3. Tolerance of Bad Data Libraries

Some bad data libraries cause the scattering cosine in a collision to be greater than unity, and MCNPX terminates with a "bad trouble" error. Now the "fatal" option may be used in the MCNPX execution line so that cosines >1 merely cause warning messages (JL/GWM/JSH).

3.4.4. Improve Annoying Messages

- Fix annoying high-energy messages that are issued repeatedly when negative cross sections are found in the physics model region. The single message, "negative x-s in sighad for the following target nuclide" now is issued at the first occurrence (GWM).

- Remove the meaningless message "**** cross sections taken from barpol.dat ****" (GWM).

- Provided clearer error messages for SI/SP with large lattices (JSH).

3.4.5. SGI Installation
The DEC compiler directive no longer is needed when compiling MCNPX on SGI platforms (GWM).

4.0. MCNPX 2.5.d CORRECTIONS

4.1. Significant Problem Corrections

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

4.1.1. DXTRAN Mesh Tally Type 4
The DXTRAN mesh tally type 4 has been incorrect in all previous versions because the DXTRAN tracks were plotted as going out in random directions (EJP/GWM).

4.1.2. Incorrect Antineutron and Antiproton Table Range Heating
Heating tallies have incorrect contributions from antineutrons and antiprotons in the neutron and proton data table energy range. Fortunately, antineutrons and antiprotons are rare, and the amount of incorrect heating is small. Antineutrons and antiprotons correctly use physics models and deposit energy by a collision estimator energy balance at each collision. Incorrectly, they also have contributed (in all previous versions) a track-length heating multiplied by the heating number of the last neutron (or proton) in the same nuclide. This incorrect additional heating occurs only for energies below the neutron or proton data table energy range. Because antiparticles decay quickly, the track lengths are short and the heating contribution small. Whenever the incorrect heating occurs, the spurious error message, "Warning. Wrong cross section used." is displayed. A cash award of $2 was made to Martyn Swinhoe, NIS-5, LANL (D-5:JSH-2003-36), for discovering this error.

4.1.3. Spontaneous Fission Multiplicities
The spontaneous fission neutron multiplicities for some nuclides have been corrected. The incorrect data was for nuclides with long half-lives for which spontaneous fission is improbable. The fission multiplicity for the main spontaneous fission nuclides ^{238}Pu, ^{240}Pu, ^{242}Pu, ^{242}Cm, ^{244}Cm, and ^{252}Cf remains correct (JSH).

4.1.4. Incorrect Detector Scores
Detectors can give incorrect answers if duplicate detector locations are found on different detector tallies. A cash award of $2 was made to Edward Waller, University of Ontario, Ontario, Canada (D-5:JSH-2003-069), for discovering this error (GWM).

4.1.5. HTAPE3X Damage Energy
An error in the HTAPE3X equation for epsilon (MCNPX manual, p. 220) caused a small change in the calculated damage energy (EJP).

4.2. Irritating Problems

The following problems do not cause incorrect answers. In some cases, MCNPX will crash, and in others, the desired functionality simply is absent.

4.2.1. Problems Calculating Tally Segment Volumes

A PVM crash was traced to an old MCNP error in which the code attempts to calculate tally segment volumes for point detectors and pulse-height tallies. Further, tally segment surface areas and tally segment volumes were not calculated for particle types IPT >3. A cash award of $2 was made to Anthony Zukaitis, Bechtel Nevada-LAO (D-5:JSH-2003-065), for discovering this error (GWM/JSH).

4.2.2. Unexpected Termination for Small Time Cutoffs

If very small time cutoffs were used (CUT:*pl* Ecut Tcut), then MCNPX would terminate with the “bad trouble” error: “Event distance = zero.” The inability to handle a negative distance-to-time cutoff has been present in all previous MCNPX versions. These particles now are terminated correctly as “lost to time cutoff.” A cash award of $2 was made to Kin Yip, BNL (D-10:JSH-2003-37), for discovering this error.

4.2.3. Crash with Incorrect Error Message

A typographical error (format word count) in the error message “unresolved resonances use variance reduction with f8” caused a crash. A cash award of $20 was made to Steven C. van der Marck, NRG, Petten, The Netherlands (D-5:JSH-2003-052), for discovering this error.

4.2.4. Crash with Lattice Fill

Some problems with repeated structures/lattices were traced to inadequate storage space being set aside for the lattice fill. A cash award of $20 was made to Miguel Embid Segura, CIEMAT, Madrid, Spain (D-5:JSH-2003-068), for discovering this error (GWM).

4.2.5. DXTRAN with Repeated Structures

When DXTRAN is used with repeated structures/lattices, the coordinates of particles leaving the DXTRAN sphere may be incorrect, causing a crash or incorrect weight cutoff game. A cash award of $2 was made to David Lawrence, NIS-1, LANL (D-5:JSH-2003-088), for discovering this error (GWM).

4.2.6. TECPLOT Plot with Total Bin

Tecplot crashed when a total bin was specified due to improper format statements in RDMCTAL in GRIDCONV (LSW).

4.2.7. System Problems

Some systems had problems with various F90 constructs that do not affect most other systems. Consequently, the following changes were made.

- Allocation of floats to integer, such as ara = 0, set to floats: ara = zero (GWM).

- Swept DAC variables, in some cases, now allocate from position 0 (GWM).

- The initialization for KTC was incorrect for MPI and PVM (GWM).
- The MPI ifdef in GETEXM should have been only for the GETEXM in MCNPF directory (GWM).
- A workaround was added for a PGF90 3.3 Linux compiler bug, thus preventing proper writing to RUNTPE (GWM).
- A workaround was added for a bug in some Sun compilers (routine NEXTIT), thus preventing proper reading of the MPLOT card (JSH).

4.3. Completely Harmless Problems

The following problems are completely harmless on most systems.

4.3.1. Bad Parameter Values

Two unused parameters in CEM include statement double.h (dp257m3 and dp59m3) were incorrect. A $2 cash award was made to Tom Jordan, EMPI, Gaithersburg, Maryland (X-5:JSH-2003-032), for discovering this error (FXG).

4.3.2. Protect from Bad Square Roots

Protect from bad square roots (CEM routine CEMSTAT) (GWM).

4.3.3. Do Not Use Exit Call

Use stop instead of exit (CEM routine QINTS) (GWM).

4.3.4. Bad F77 Constructs

Some obsolete F77 constructs where lines were assumed to be continued at column 72 were corrected (HTAPE3X include COM32B.h) (Gary Grim, P-23, LANL).

5.0. FUTURE WORK

- Plotting of physics model total and absorption cross sections
- Forced collisions for neutral particles extended to physics models
- Cinder90 capabilities
  - Delayed neutrons physics models
  - Delayed gamma physics models
  - Transmutation
- Pulse-height tallies with variance reduction
- Lattice tally contour plotting
- Intel computer support
- 64-bit integer support
- Improved high-energy physics with the LAQGSM model
- Secondary particle angle biasing for isotropic distributions
- Neutral particle perturbation techniques extended to physics model region
- Heavy-ion tracking and interactions
- Detectors and DXTRAN for all neutral particles at all energy ranges
- A capability to continue runs that write HTAPE files
- Interactive tally and cross-section plotting

- Integration of HTAPE tallies directly into MCNPX
- Criticality
  - Externally driven sources
  - Improved stability of eigenfunctions
  - Enhanced efficiency for parallel kcode calculations
- CAD link