MCNPX Features for 2006

by

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MCNPX Features for 2006

- MCNPX Overview

- History of MCNPX

- User Base

- Features for 2006

- Future of MCNPX

MCNPX Overview

- Monte Carlo radiation transport code
  - Extends MCNP4C to virtually all particles and energies
  - 34 particles (n,p,e, 5 leptons, 11 baryons, 11 mesons, 4 LI)
  - Continuous energy (roughly 0-100 GeV)
  - Data libraries below ~ 150 MeV (n,p,e,h) & models otherwise

- General 3-D geometry
  - 1st & 2nd degree surfaces, tori, 10 macrobodies, lattices

- General sources and tallies
  - Interdependent source variables, 7 tally types, many modifiers

- Supported on virtually all computer platforms
  - Unix, Linux, Windows, OS X (parallel with MPI)

History of MCNPX
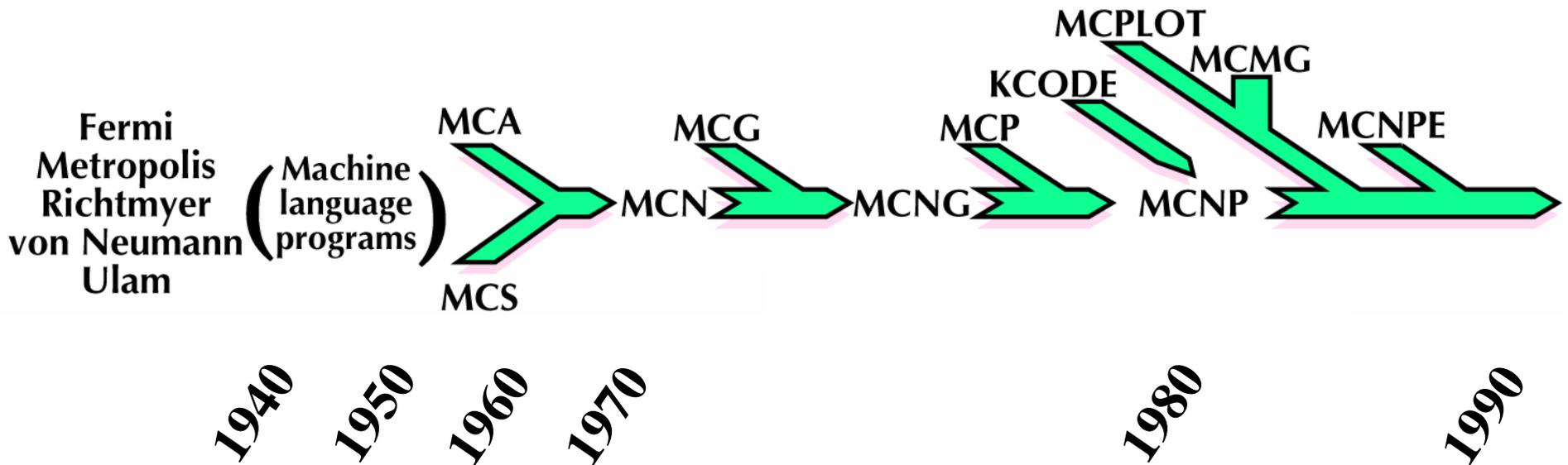
History of MCNPX
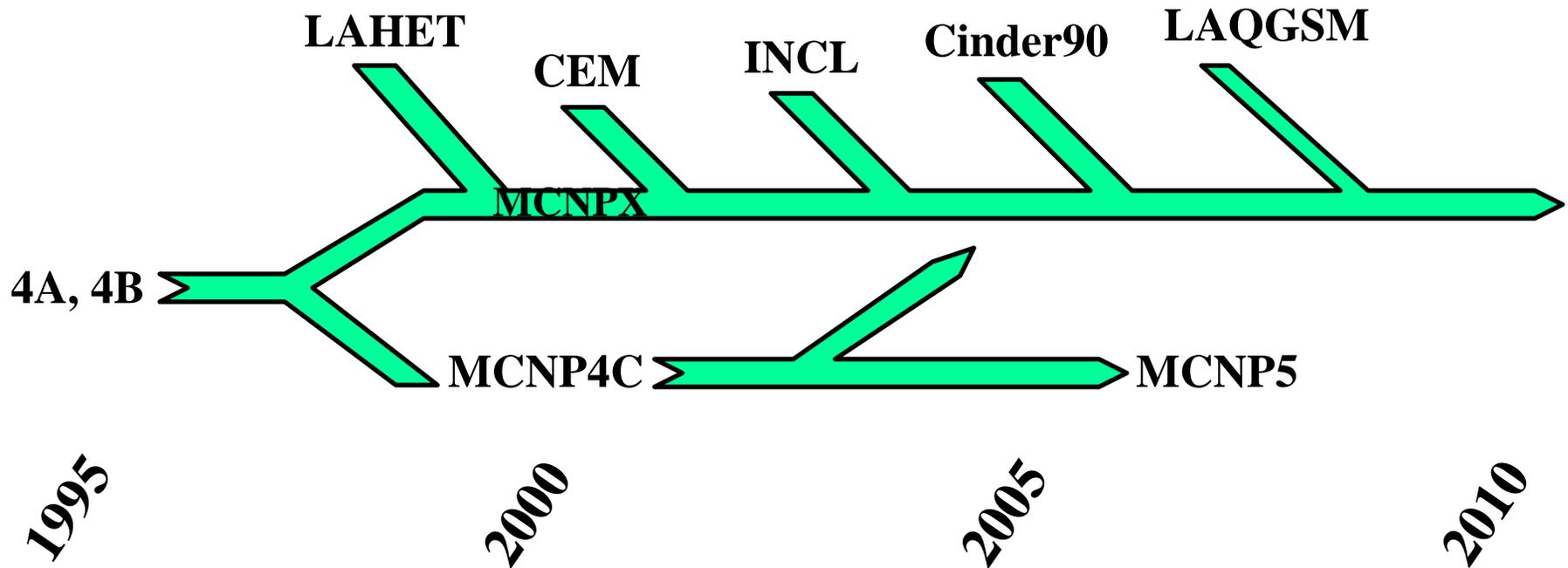
History of MCNPX

1992-1993   LAHET and Superhet
   Superconducting Super Collider
1994-1995   Start of the APT program
Version 1.0   April 22, 1997
Version 2.0   October 1, 1997
Version 2.1.3   April 17, 1998
   HISTP writing, compatible with HTAPE, collisional energy loss model
Version 2.1.4   July 24, 1998
   Mesh & radiography tallies, gridconv, bertin & phtlib binary support
Version 2.1.5   **Nov 14, 1999**
   CEM, HTAPE3X, User's Manual, Beta test team
Version 2.1.6   September 14, 1999
   Proton libraries (internal user only)
Version 2.3.0   **April 27, 2002**

History of MCNPX

Version 2.4.0   **August 01, 2002**
    Update to MCNP4C3, F90, Windows PC, New user's manual

Version 2.5.C   April, 2003
    MPI Multiprocessing, Mix & Match, CEM2K

Version 2.5.D   August, 2003
    INCL4/ABLA physics models, Multiple particles on SDEF card, READ card

Version 2.5.E   February, 2004
    MPI KCODE speedup, 64-bit integers, G5 support, 2-D color contour plots

Version 2.5.0   **March, 2005**
    Mesh tally contour plots, Pulse-height tally with VR, PN improvements

Version 2.6.A   December, 2005
    Transmutation, Long file names, STOP card

Version 2.6.B   June, 2006
    CEM 03, new PHTLIB, predictor-corrector for burnup

Version 2.6.C   December, 2006
    Spherical weight windows, delayed particle production

User Base

- ~2500 users world wide
  - Provide 6-8 workshops per year (4-6 US, ~2 international)
  - 150 workshop participants per year
  - Access to RSICC/NEA released versions only
    - http://www-rsicc.ornl.gov/ (C00730) 2.5.0
    - http://www.nea.fr/html/dbprog/ (CCC-0715) 2.4.0
  - Limited access to MCNPX web site
    - http://mcnpx.lanl.gov (some documentation)

- ~2000 registered Beta Testers
  - Full access to MCNPX web site
  - Access to intermediate versions
  - Increased user support

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Application	# Groups	Percent
Medical (BNCT, proton therapy, etc.)	**50**	**15**
Spacecraft, Cosmic Rays, SEE, propulsion	**42**	**12**
Detectors, experiments, Threat Reduction	**39**	**11**
ATW, ADS, Energy Amplifiers	**37**	**11**
Fuel cycles, beginning to end, including storage	**32**	**9**
Accelerator Shielding and Health Physics	**28**	**8**
Theoretical Physics	**23**	**7**
Neutron Production for Scattering	**21**	**6**
Isotope Production	**14**	**4**
Radiography	**12**	**4**
MCNPX/MCNP code development	**11**	**3**
Homeland Security	**10**	**3**
Materials studies (IFMIF)	**6**	**2**
Radioactive Ion Beams	**5**	**1**
Irradiation Facilities	**4**	**1**
Neutrino Targets	**4**	**1**
Light Sources, electron machines	**3**	**1**

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Features for 2006 – Version 2.6.A

- BURN card - transmutation using Cinder90
  - M. Fensin's paper in session Best of RPSD 2006 - I

- Long file names (40 vs. 8 characters)

- STOP card - terminate tallies at desired precision

- Corrections/enhancements/extensions
  - Proton step size control (HSTEP on M card)
  - New $S(\alpha,\beta)$ scattering law
  - Differential data tallies extended to table physics
  - Separate printout of induced fission multiplicity

BURN Card


```
Burn 7 fuel pins surrounded by H2O in a hex lattice
1   1  -8.3     -1      u=1 imp:n=1   vol=192.287        $ Fuel
2   8  -6.5    1 -2     u=1 imp:n=1                       $ Clad
3   9  -0.7      2      u=1 imp:n=1                       $ Water
100 9  -1.8     -3  u=8 lat=2 imp:n=1 fill=-2:2 -2:2 0:0
                        8 8 8 8 8
                         8 8 1 1 8
                          8 1 1 1 8
                           8 1 1 8 8
                            8 8 8 8 8
101  0              -4           imp:n=1 fill=8
102  9  -1.8     4 -5            imp:n=1
103  0              5            imp:n=0

1 rcc 0  0 0   0 0 365   0.4095
2 rcc 0 0 -1   0 0 367   0.4750
3 rhp 0 0 -1   0 0 367   0.6565 0  0
4 rhp 0 0 -1   0 0 367   0 1.895  0
*5 rhp 0 0 -1.1  0 0 367.2  0 1.896 0

BURN  TIME=50,500
      MAT=1
      POWER=0.066956
      PFRAC=1.0,1.0
      OMIT=1,6,6014,7016,8018,9018,90234,91232
      BOPT=1.0, 4
m1    8016.60c   2.0  92235.60c  0.01  92238.60c  0.99
m8    40000.60c  1.0
m9     1001.60c  2.0  8016.60c  1.0
mt9   lwtr.01t
kcode 100 1.0 10 50
ksrc  0 0 150 1.313 0 150 -1.313 0 150 0.6565 1.137 150
      0.6565 -1.137 150 -0.6565 1.137 150 -0.6565 -1.137 150
```
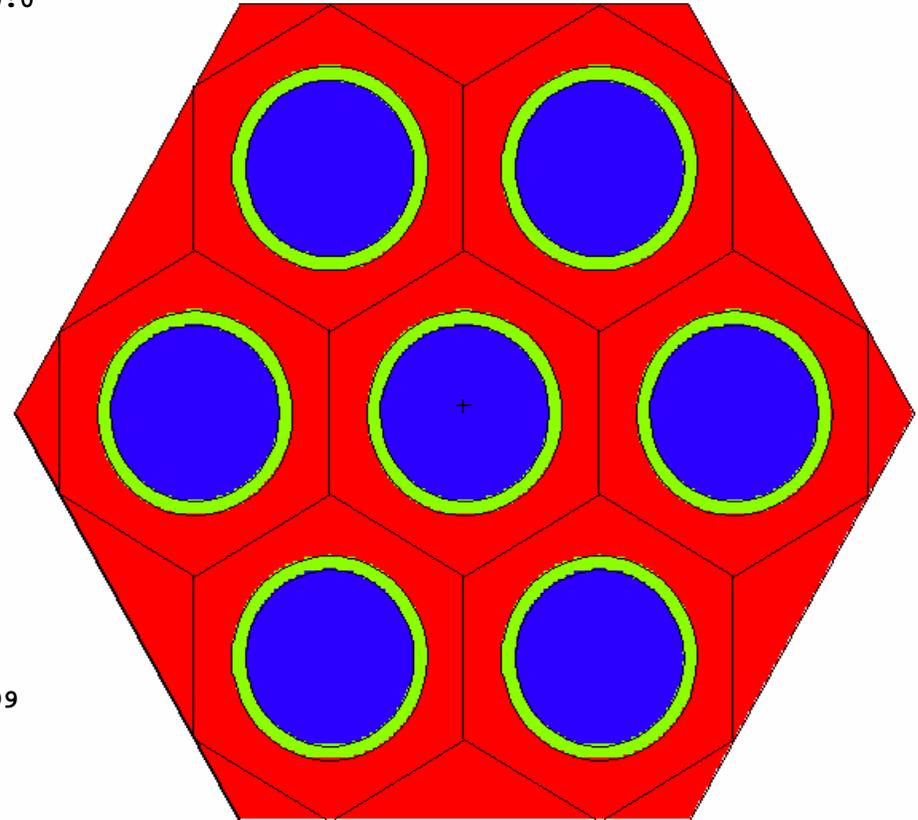
1burnup summary table by material   **print table 210**

nuclides with atom fractions below 1.000E-10 for a material are zeroed and deleted from print tables after t=0

neutronics and burnup data

step	duration (days)	time (days)	power (MW)	keff	flux	ave. nu	ave. q	burnup (GWd/MTU)
0	0.000E+00	0.000E+00	6.696E-02	0.99763	3.641E+14	2.449	200.981	0.000E+00
1	5.000E+01	5.000E+01	6.696E-02	1.00012	3.701E+14	2.554	203.154	2.383E+00
2	5.000E+02	5.500E+02	6.696E-02	0.85037	4.638E+14	2.869	209.385	2.621E+01

…

actinide inventory for sum of materials at end of step 2, time 5.500E+02 (days), power 6.696E-02 (MW)

no.	zaid	mass (gm)	activity (Ci)	sp. act. (Ci/gm)	atom den. (a/b-cm)	atom fr.	mass fr.
1	92234	3.465E-04	2.154E-06	6.217E-03	4.636E-09	2.577E-07	2.533E-07
2	92235	3.935E-01	8.506E-07	2.161E-06	5.244E-06	2.914E-04	2.877E-04
3	92236	1.789E+00	1.157E-04	6.467E-05	2.374E-05	1.319E-03	1.308E-03
4	92237	7.849E-03	6.405E+02	8.160E+04	1.037E-07	5.763E-06	5.739E-06
5	92238	1.355E+03	4.553E-04	3.361E-07	1.782E-02	9.905E-01	9.904E-01
6	92239	1.539E-03	5.158E+04	3.351E+07	2.016E-08	1.121E-06	1.125E-06

…

| 14 | 94242 | 1.117E+00 | 4.418E-03 | 3.954E-03 | 1.446E-05 | 8.034E-04 | 8.169E-04 |
| | totals | 1.368E+03 | 1.041E+05 | 7.610E+01 | 1.799E-02 | 1.000E+00 | 1.000E+00 |

…

nonactinide inventory for sum of materials at end of step 2, time 5.500E+02 (days), power 6.696E-02 (MW)

no.	zaid	mass (gm)	activity (Ci)	sp. act. (Ci/gm)	atom den. (a/b-cm)	atom fr.	mass fr.
1	6012	2.336E-06	0.000E+00	0.000E+00	6.096E-10	1.638E-08	1.186E-08
2	6013	1.057E-02	0.000E+00	0.000E+00	2.545E-06	6.839E-05	5.366E-05
3	8016	1.891E+02	0.000E+00	0.000E+00	3.702E-02	9.946E-01	9.599E-01
4	8017	1.405E-02	0.000E+00	0.000E+00	2.588E-06	6.954E-05	7.132E-05

…

| 16 | 60145 | 3.469E-01 | 1.426E-14 | 4.112E-14 | 7.497E-06 | 2.014E-04 | 1.761E-03 |
| | totals | 1.970E+02 | 8.830E+01 | 4.483E-01 | 3.722E-02 | 1.000E+00 | 1.000E+00 |

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Long File Names

E:\MCNPX\scratch>.\mcnpx inp=test_long_names.txt na=test_long_names.
 mcnpx   ver=26bc1 ld=Sat Jul 01 08:00:00 MST 2006   11/12/06 20:08:04

…
dynamic storage =   0 words,   0 bytes.   cp0 = 0.00
 run terminated when   10 particle histories were done.
 dump   2 on file test_long_names.r   nps =   10 coll =   0
                 ctm =   0.00   nrn =   40
 mcrun is done

E:\MCNPX\scratch>dir

Directory of E:\MCNPX\scratch

11/12/2006 08:08 PM   <DIR>   .
11/12/2006 08:08 PM   <DIR>   ..
09/11/2006 03:23 PM   6,574,080 mcnpx.exe
11/12/2006 08:08 PM   22,513 test_long_names.d
11/12/2006 08:08 PM   25,510 test_long_names.o
11/12/2006 08:08 PM   401,342 test_long_names.r
08/04/2006 01:21 PM   481 test_long_names.txt
           5 File(s)   7,023,926 bytes
           2 Dir(s) 31,759,495,168 bytes free

STOP Card

14 MeV neutrons in water - test STOP card
```
c     cell cards
1     1   -1.  -1 IMP:N=1
2     0        1 IMP:N=0


1     so 30.0


m1     1001.60c 2. 8016.60c 1.
mt1    hh2o.20t
xs1    hh2o.20t 0.998623 ct00 0 1 1 1237501 0 0 2.530E-08
sdef   erg=14.1
e0     1.00000E-11 625log 1.44544E+01
vol       1.
f44:n    1
f141:n   1
STOP     F44 .01 NPS 10000 CTME 10.0
```
OUTPUT FILE

```
1tally fluctuation charts
```

	tally 44					tally 141				
nps	mean	error	vov	slope	fom	mean	error	vov	slope	fom
1000	5.6661E+01	0.0144	0.0031	10.0	489705	3.7459E-01	0.0354	0.0003	0.0	81225
2000	5.6824E+01	0.0103	0.0016	10.0	468574	3.7000E-01	0.0254	0.0002	10.0	77294
3000	5.7028E+01	0.0083	0.0010	10.0	477186	3.6737E-01	0.0209	0.0001	10.0	75590

```
*****************************************************************************************
dump no.   2 on file stop.r    nps =        3000   coll =         599417   ctm =    0.03
```

New S(α,β) Treatment

```
14 MeV neutrons in water - test S(alpha,beta)
c     cell cards
1     1  -1.  -1 IMP:N=1
2     0        1 IMP:N=0


1     so 30.0


m1      1001.60c 2. 8016.60c 1.
mt1     hh2o.20t  $ Use lwtr.01t for previous treatment
xs1     hh2o.20t 0.998623 ct00 0 1 1 1237501 0 0 2.530E-08
nps     1000000
sdef  erg=14.1
e0    1.00000E-11 625log 1.44544E+01
vol     1.
f44:n   1
f141:n  1
```

New S(α,β) Treatment

Neutron flux in the water

2.5.0/lwtr.01t

2.6.C/new S(α,β) file
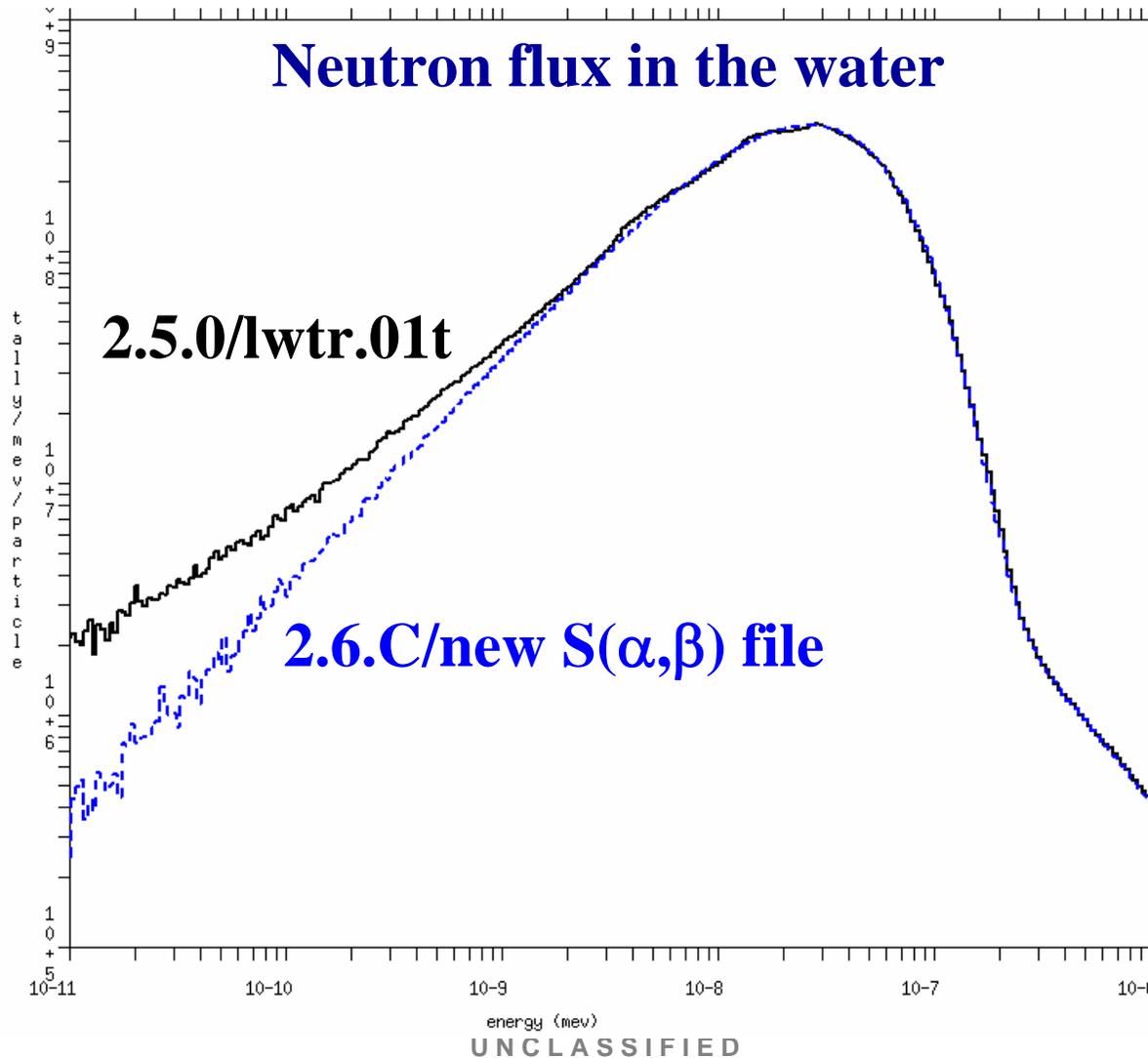
Features for 2006 – Version 2.6.B

- Transmutation improvements
  - M. Fensin's paper in Burnup/Depletion Modeling
  - Predictor/corrector
  - Automatic selection of FP dist. (thermal, fast, high)

- CEM INC model upgrade (from 2K to 03)

- FIELD card–planetary gravity effects for neutrons

- Corrections/enhancements/extensions
  - New photon emission data: PHTLIB
  - Geometry plot basis vectors
  - Extend ZAID identifiers

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CEM Upgrade

Secondary particle production

1 GeV protons into Fe-56
```
1     1   -7.86 -1 IMP:N=1
2     0         1 IMP:N=0

1     so 1.0

mode  n h
m1    26056.24c 1.
nps   200000
sdef  erg=1000 par=h
PHYS:N 1001.0
LCA   7j -2 1 $ Use CEM
e0    1 199log 1000
c0    0 1
f1:n  1
f11:h 1
prdmp 2j 1
```

2.6.C neutrons

2.6.C protons

2.5.0 protons

2.5.0 neutrons
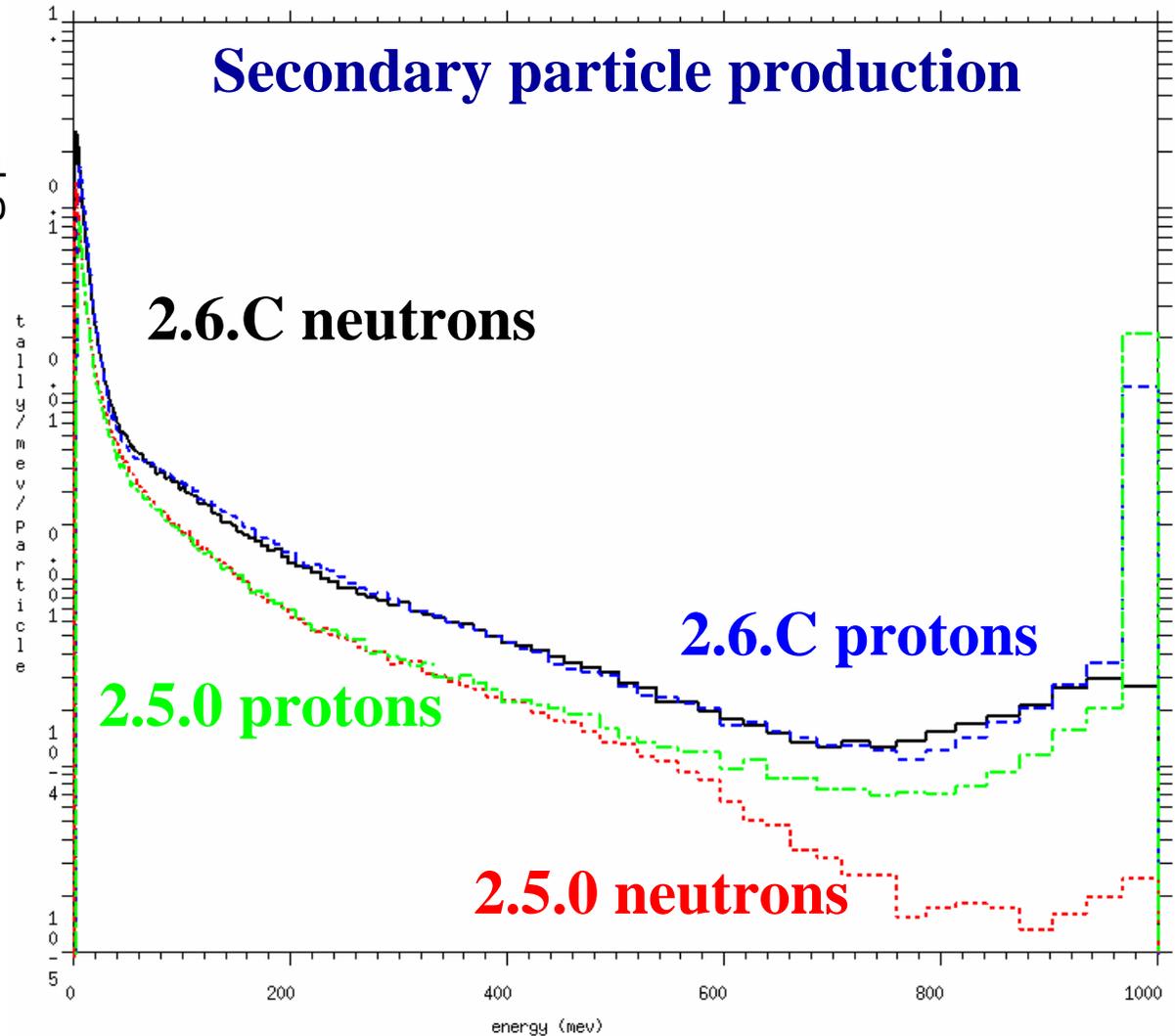
CEM Upgrade

Light-product yields (A<30)

Model	Proton energy (MeV)					
	300	500	750	1000	1500	2600
BERTINI	1035	26.1	50.5	13.8	4.93	3.35
ISABEL	---	256	49.1	17.0	5.99	4.02
INCL	233	215	51.5	38.1	26.1	12.1
CEM2K	---	12.6	21.1	7.83	4.87	4.02
CEM03	13.0	2.23	1.32	1.49	1.58	1.72

Heavy-product yields (A>30)

Model	Proton energy (MeV)						Ave. Dev.
	300	500	750	1000	1500	2600	
BERTINI	2.24	2.29	2.75	2.86	3.16	3.20	4.37
ISABEL	3.75	2.85	3.02	2.63	2.85	3.01	4.24
INCL	4.72	3.24	3.14	3.13	3.35	3.54	7.14
CEM2K	2.74	2.54	2.62	2.76	2.92	3.20	3.55
CEM03	1.84	1.89	1.89	1.92	2.04	3.17	2.26

Mean-squared deviation factors between model predictions and experimental data measured at ITEP.

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FIELD Card

5 GeV protons into Martian soil with gravity reflection
```
1      1 -1.0          -1          imp:n=1
100    2 -1.35e-5      -101 +1     imp:n=1
101    2 -1.28e-5      -102 +101   imp:n=1
102    2 -1.22e-5      -103 +102   imp:n=1
103    2 -1.14e-5      -104 +103   imp:n=1
104    2 -1.08e-5      -105 +104   imp:n=1
105    2 -1.01e-5      -106 +105   imp:n=1
999    0              +106         imp:n=0

1      so 339000000.0
101    so 339060000.0
102    so 339110000.0
103    so 339180000.0
104    so 339240000.0
105    so 339310000.0
106    so 339380000.0

m1     8016.60c -0.6 14000.60c -0.3 26056.60c -0.1
m2     6000.60c -0.27 7014.60c -0.02 8016.60c -0.70 18000.35c -0.01
FIELD GCUT=0.1320 GPAR=1 GRAD=3393.0 GSUR=106
mode   h n p z / d t s a
lca    8j 1 $ Use CEM
sdef   par=9 erg=5000 sur=106 nrm=-1
nps    10000
print
phys:n 5010 j j j 20
e11    0. 1024i 10. 5000.
fu11   0. 8016.00051 8016.00052 8016.00053 8016.00102  8016.
       14028.14027 14028.14026 14028.13027 14028.13026 14000.
       26056.00051 26056.00052 26056.00053 26056.00102 26056.
f11:p 1
ft11  tag 1
e21    1e-10 99log 1e-7
f21:n 105
```

Undocumented Feature

FIELD Card

Neutron current at top of atmosphere

With gravity

Without

Features for 2006 – Version 2.6.C

- Transmutation improvements
  - Support for continue-runs
  - Printing of reaction rates sent to Cinder90
  - Reduced memory requirements

- Spherical weight windows

- Delayed neutrons & gammas
  - ~1000 nuclides treated with gamma line data

- Photon tally tagging

- Model treatment for library absorption reactions

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Spherical Weight Windows


```
Disk of 10 MeV photons into 95cm H2O surrounding 3cm HEU
1  1  -19.0   -1    imp:p=1
2  2  -1.0    +1 -2 imp:p=1
3  0          +2 -3 imp:p=1
4  0             -3 imp:p=0


1 sph 0 0 0   3
2 sph 0 0 0   100
3 sph 0 0 0   200


mode p
sdef erg=10 pos -105 0 0 rad=d1 axs=1 0 0 ext=0
     vec=1 0 0 dir=d2
si1  0 10
sp1  -21 1
si2  0 1
sp2  0 1
m1   92235 .5 92238 .5
m2   1001 2 8016 1
nps 100000
f4:p 1
wwg 4 0
mesh geom rpt origin=0 0 0 ref=-99 1 1 axs 1 0 0 vec 0 1 0
     imesh  101.   iints  20
     jmesh  .25 .5 jints  4 8
     kmesh  1      kints  1
c    wwp:p  4j -1    $ Add this card to use WW
```

Polar axis
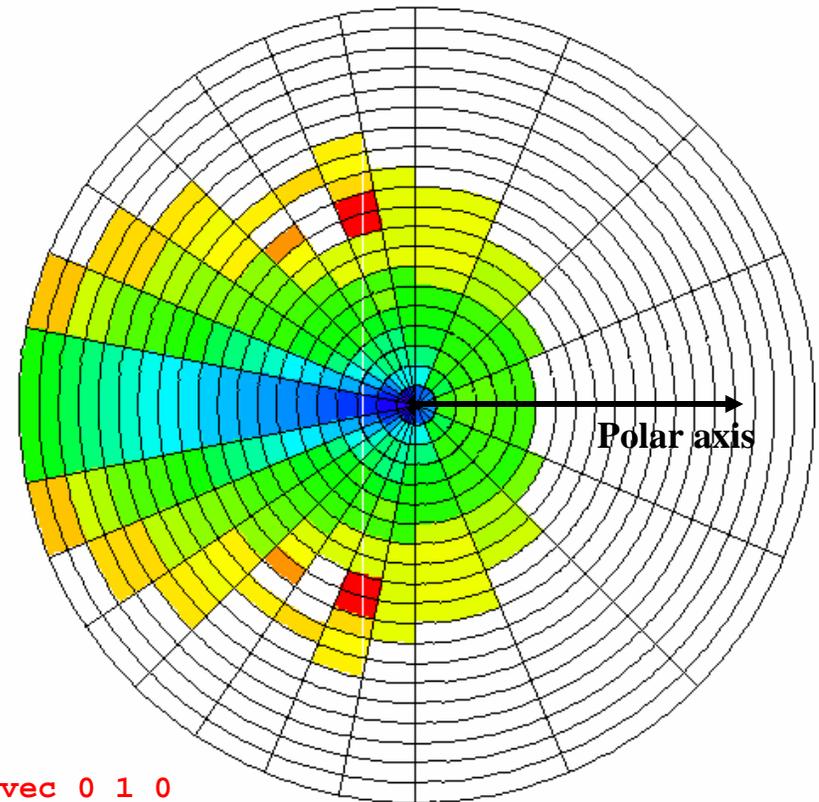
Delayed Neutrons and Gammas

```
Delayed gammas from Watt fission in U-235
1      1 -18.9  -1 IMP:N=1
2      0          1 IMP:N=0


1      so 0.01975


mode   n p
m1     92235.60c 1.
nps    20000000
sdef   erg=d1 par=n
sp1    -3
phys:p 5j -1
e0     0. 1024i 10.0
t0     .001e8 .01e8 .1e8 1e8 10e8 100e8
f1:p   1
```

Delayed Neutrons and Gammas

Delayed Neutrons and Gammas

Comparison to Measured Data

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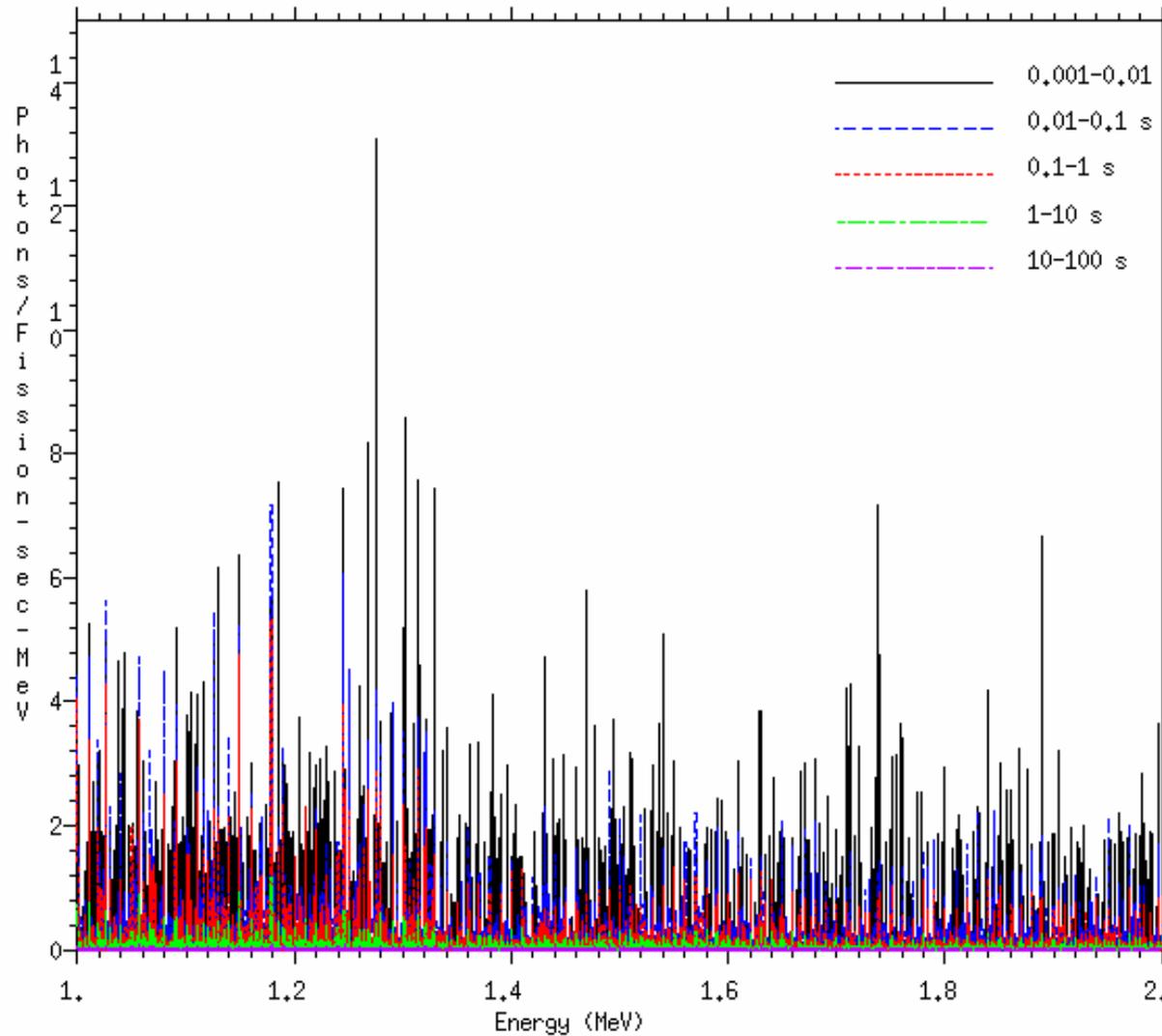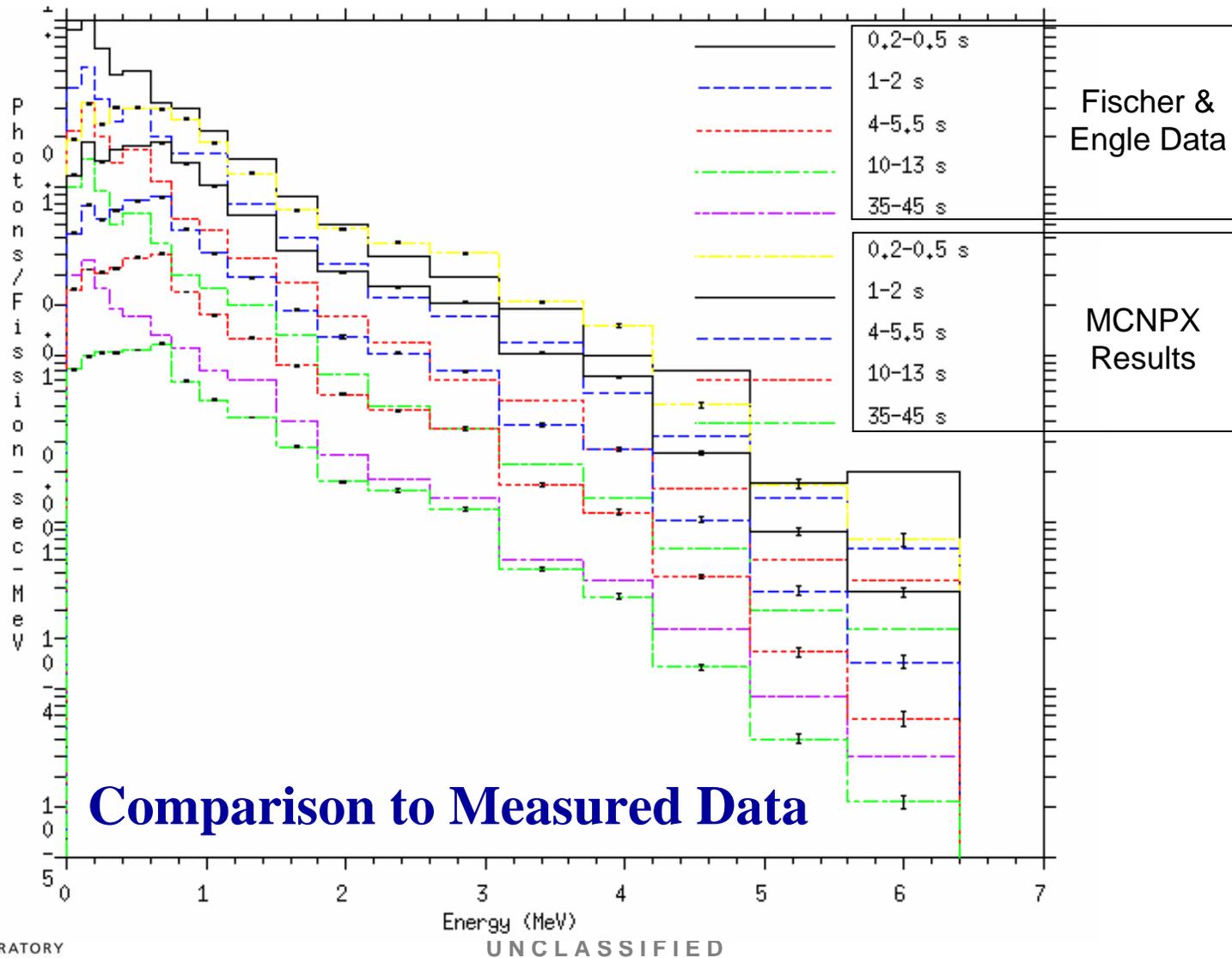
Photon Tally Tagging

```
5 GeV protons into Martian soil with photon tagging
1     1 -1.0        -1        imp:n=1
100   2 -1.35e-5    -101 +1   imp:n=1
101   2 -1.28e-5    -102 +101 imp:n=1
102   2 -1.22e-5    -103 +102 imp:n=1
103   2 -1.14e-5    -104 +103 imp:n=1
104   2 -1.08e-5    -105 +104 imp:n=1
105   2 -1.01e-5    -106 +105 imp:n=1
999   0            +106       imp:n=0

1     so 339000000.0
101   so 339060000.0
102   so 339110000.0
103   so 339180000.0
104   so 339240000.0
105   so 339310000.0
106   so 339380000.0

m1    8016.60c -0.6 14000.60c -0.3 26056.60c -0.1
m2    6000.60c -0.27 7014.60c -0.02 8016.60c -0.70 18000.35c -0.01
FIELD GCUT=0.1320 GPAR=1 GRAD=3393.0 GSUR=106
mode  h n p z / d t s a
lca   8j 1 $ Use CEM
sdef  par=9 erg=5000 sur=106 nrm=-1
nps   10000
print
phys:n 5010 j j j 20
e11   0. 1024i 10. 5000.
fu11  0. 8016.00051 8016.00052 8016.00053 8016.00102  8016.
      14028.14027 14028.14026 14028.13027 14028.13026 14000.
      26056.00051 26056.00052 26056.00053 26056.00102 26056.
f11:p 1
ft11  tag 1
e21   1e-10 99log 1e-7
f21:n 105
```

Undocumented Feature

# Photon Tally Tagging

Deexcitation gammas from ^{28}Si

Models for Library Interactions

```
2 MeV neutrons into He-3                    f8:n  1
1  1 -5.3540E-4  -1    imp:n=1              e8    0. 99i 2.1
2  0              1 -2 imp:n=1              ft8   PHL 1  6 1 0
3  0              2    imp:n=0              f18:n 1
                                            e18   0. 99i 2.1
                                            ft18  PHL 1 16 1 0
1  so 4.0                                   f28:n 1
2  so 100.0                                 e28   0. 99i 2.1
                                            ft28  PHL 1 26 1 0
                                            f38:n 1
mode   n h d t s                            e38   0. 99i 2.1
sdef   par=n erg=2 pos=-5 0 0 rad=d1        ft38  PHL 1 36 1 0
       axs=1 0 0 ext=0 vec=1 0 0 dir=1      f58:n 1
si1    0 3                                  e58   0. 99i 2.1
sp1    -21 1                                ft58  PHL 4 6 1 16 1 26 1 36 1 0
cut:n  2j 0 0
cut:h,d,t,s j .001
phys:n 6j 2
m1     2003.60c 1
nps    10000000
f6:h   1
f16:d  1
f26:t  1
f36:s  1
```

Models for Library Interactions

Pulse height tally from all particles

He-3

Total

Tritons

Protons
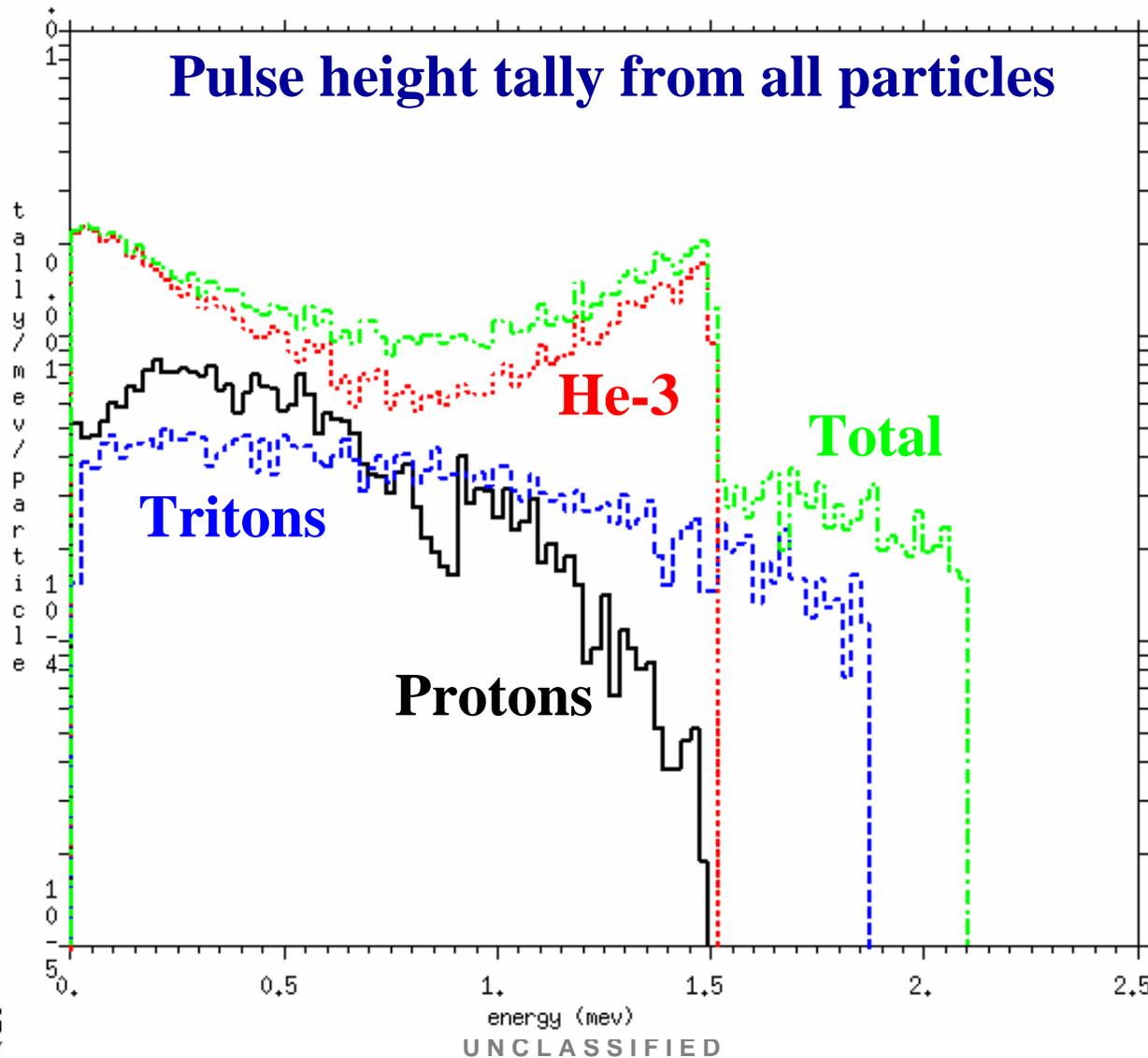
Future of MCNPX

- Possible public release of 2.6.0 (Jan. 2007)
- Version 2.6.D/2.7.A (March 2007)
  - Transmutation improvements
  - Energy and time weight windows
  - Radioactive source option
  - Photofission and delayed neutron improvements
- MCNPX and MCNP merger
  - Hope to preserve all features of both codes
  - Preliminary version by Summer 2007
  - Public release perhaps by 2008

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