Implementation of Homeland Security Features in MCNP/X

Michael R. James

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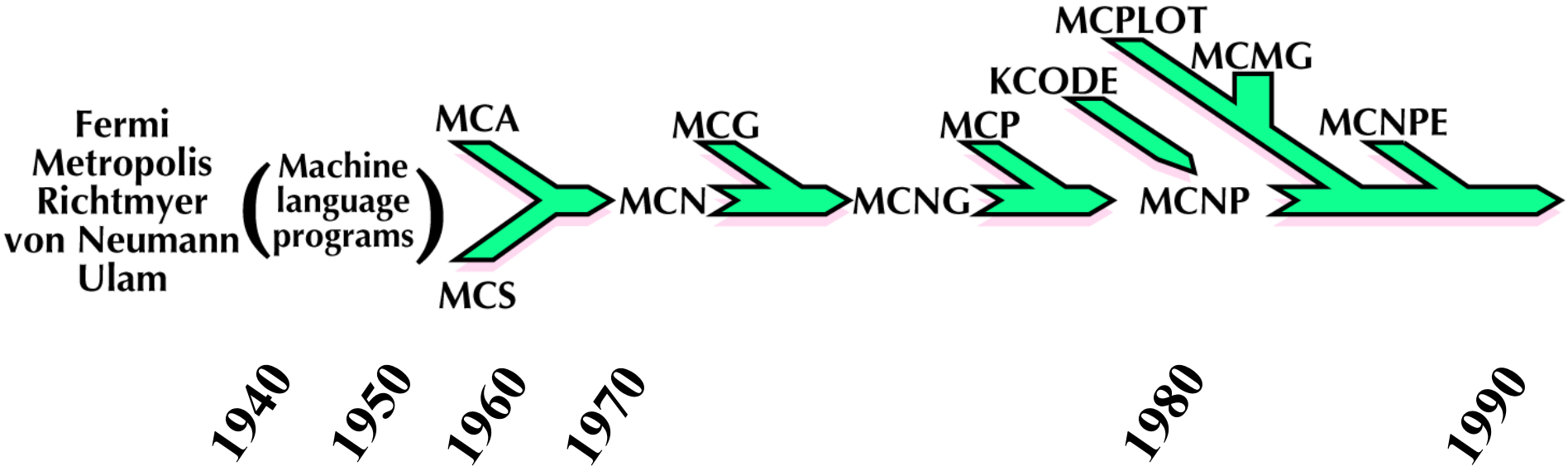
Outline

- **Overview**
- **Physics Enhancements**
  - **Photon Form Factors upgrade**
  - **NRF Libraries**
  - **Delayed Gamma Speedup**
  - **M & MX Card Enhancements**
- **Tally Enhancements**
  - **FT ROC**
  - **FT RES (upgrades, cell-based)**
  - **FT PHL (time bins, 4 fold coincidence)**
  - **Cyclic Time bins using keywords**
- **Other Enhancements**
  - **ACT card (control for DNDG)**

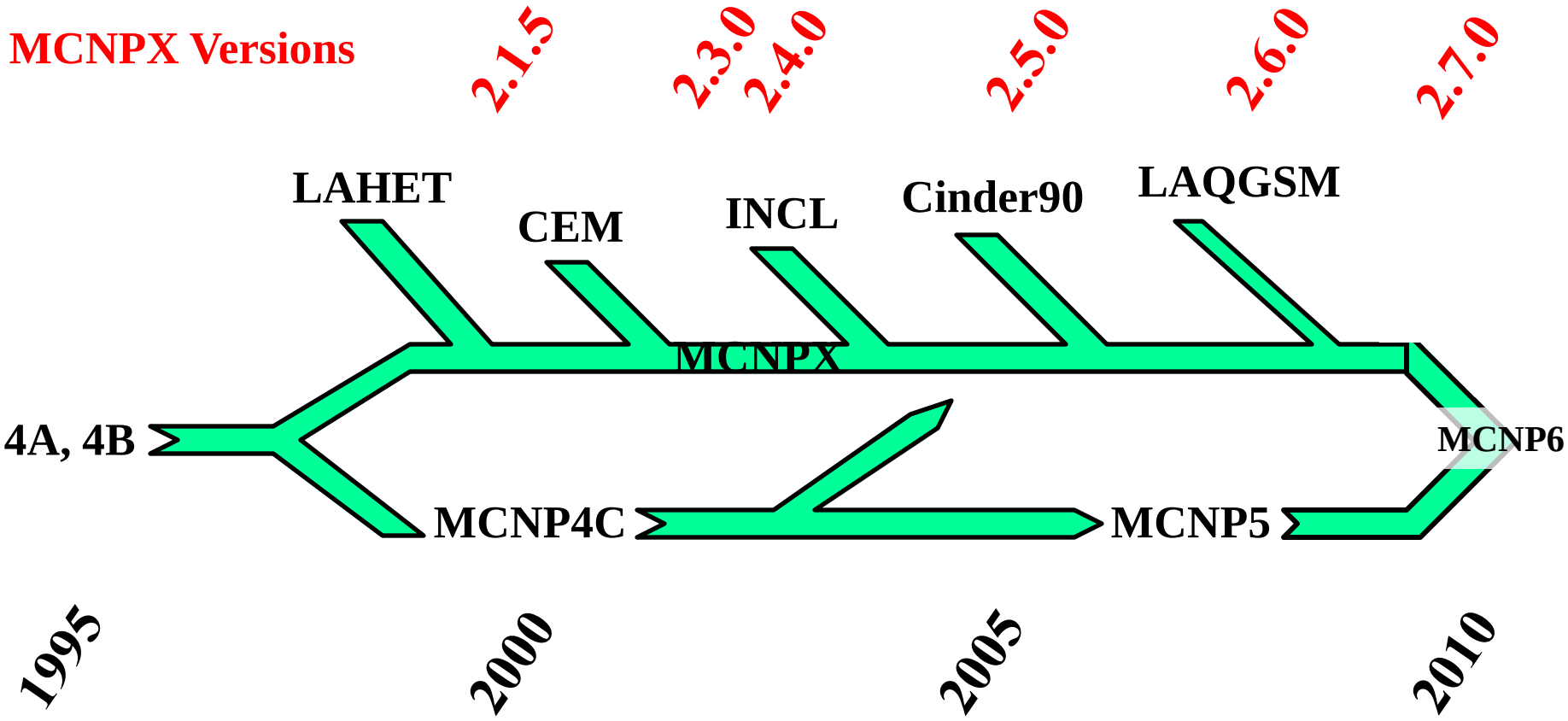
Overview – MCNP/X is a 3-D, all-particle, all-energy Monte Carlo transport code

- **Monte Carlo radiation transport code**
  - Extends MCNP4C to virtually all particles and energies
  - 34 different particle types + 2205 heavy ions
    - Neutrons, photons, electrons, protons, pions, muons, light-ions, etc.
  - Continuous energy (~0 -1 TeV/n)
  - 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)

Overview – The previous century of development



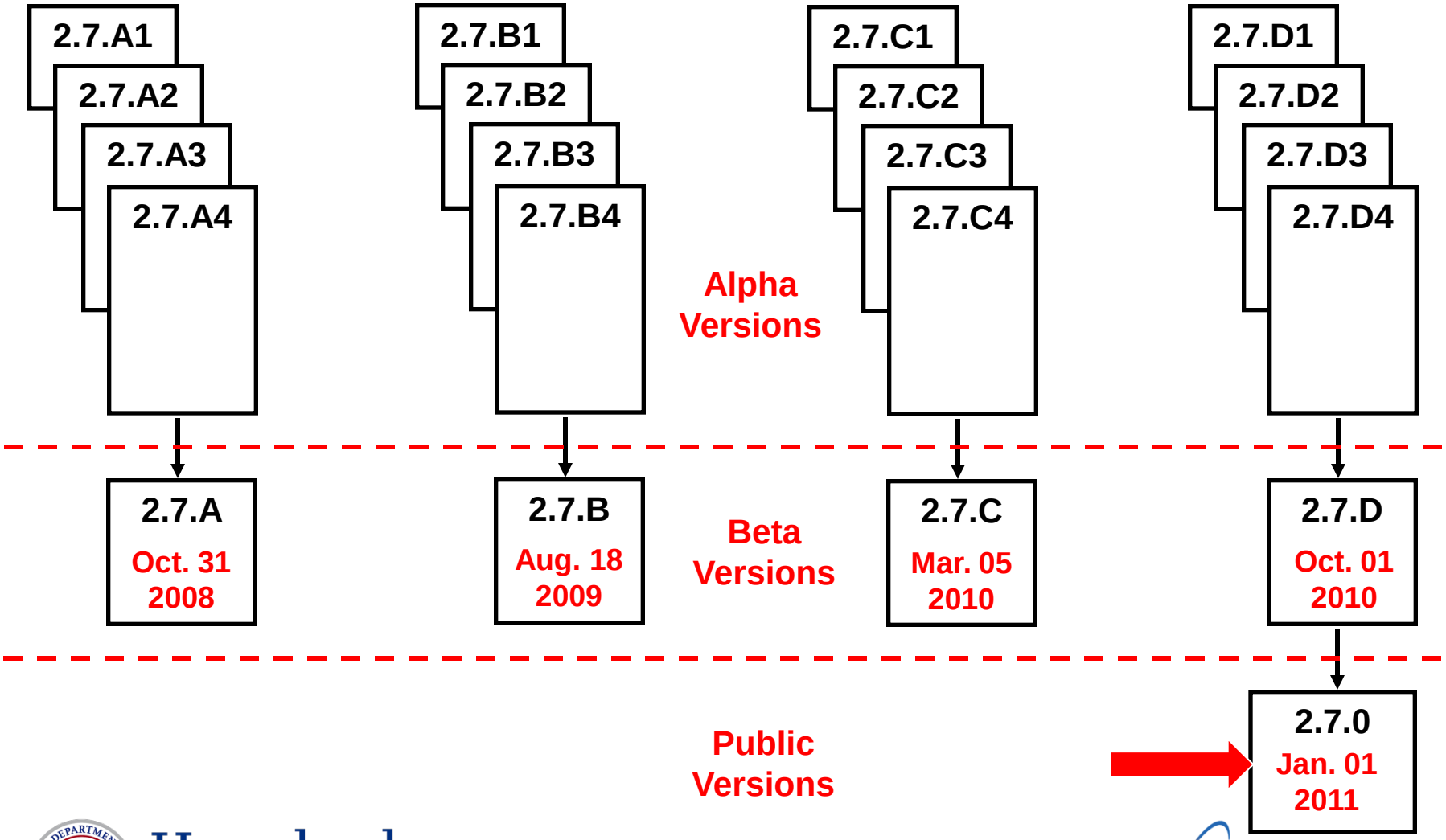
Overview – The current century of development



Overview – Resources for MCNPX users

- **~3000 users world wide**
  - Provide 6-8 workshops per year (4-6 US, 2 international)
  - 1-2 workshops per year have a HS or TR emphasis
  - Access to RSICC/NEA released versions only
    - http://www-rsicc.ornl.gov/ (C00740) 2.6.0
    - http://www.nea.fr/html/dbprog/ (CCC-0740) 2.6.0
  - Limited access to MCNPX web site
    - http://mcnpx.lanl.gov (some documentation)
- **~2000 registered Beta Users**
  - Full access to MCNPX web site
  - Access to intermediate Beta versions
  - Increased user support

Test suite enhancements – developmental versions of MCNPX



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Test suite enhancements – versions 2.7.A, 2.7.B, 2.7.C, 2.7.D

Physics Enhancements

CEM upgrade to 03.02
Adjustable stopping-power grid
LLNL photofission multiplicities
Delayed gamma exact sampling
LLNL neutron fission multiplicities
Muonic x-ray enhancements
Delayed neutron spectra
NRF data in ACE libraries
Improved photoatomic form factors
DG algorithm improvements
M & MX card enhancements

Source Enhancements

Burnup enhancements
Pulsed sources
Beam source options

Tally Enhancements

Tally tagging
LET tally option
Quality factor tally option
Cyclic tally binning
ROC curve tally option
Residual tally upgrades
Triple & quadruple coincidences
Time-dependent pulse-height tallies

Variance Reduction Enhancements

Other Enhancements

MCPLOT graphics enhancements
Activation options (ACT card)
MCPLOT tally manipulations
Nested READ cards
Feature-based memory reduction

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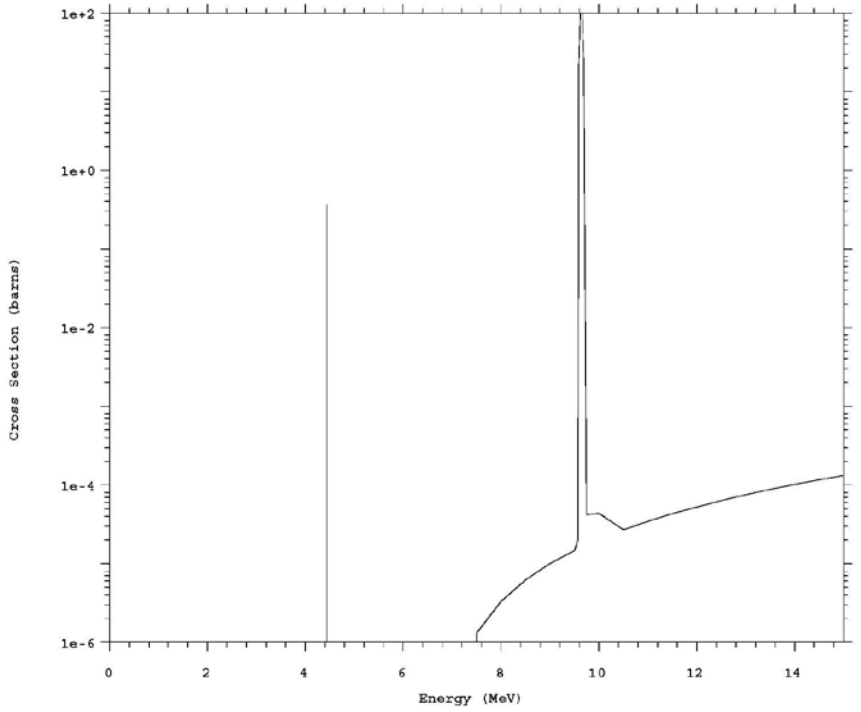
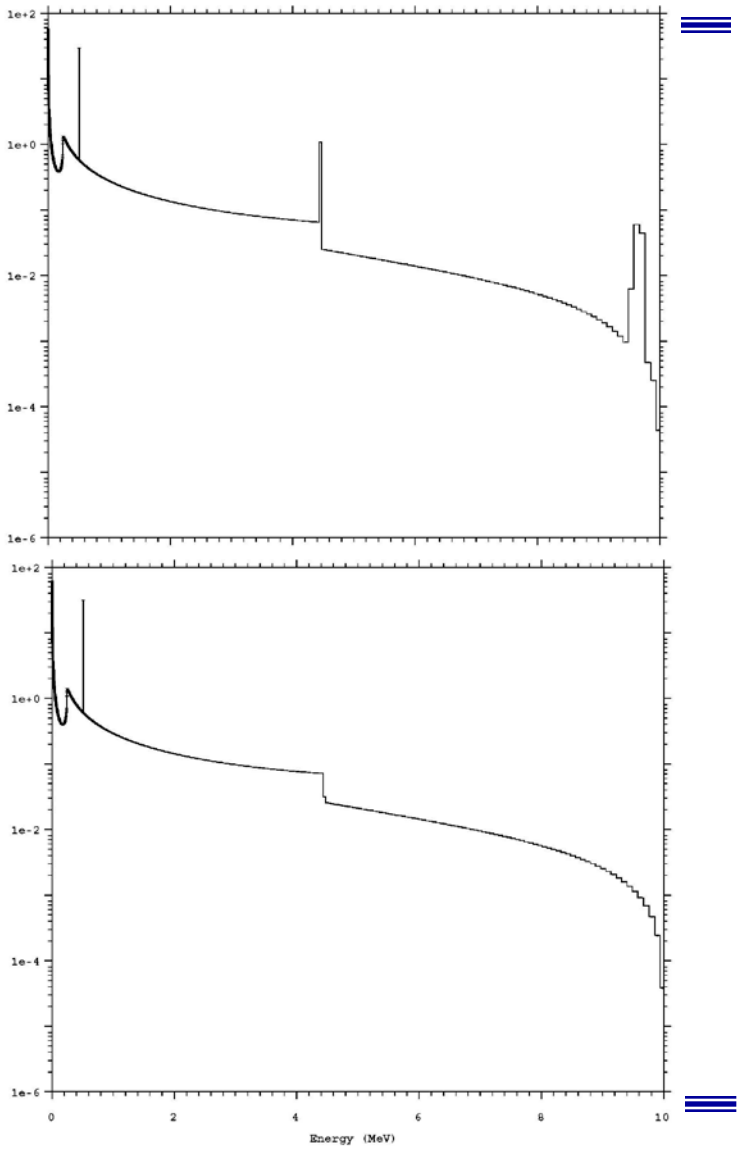
New NRF library (PN3-NRF) consists of 155 isotopes – data is undergoing verification and benchmarking

C-12

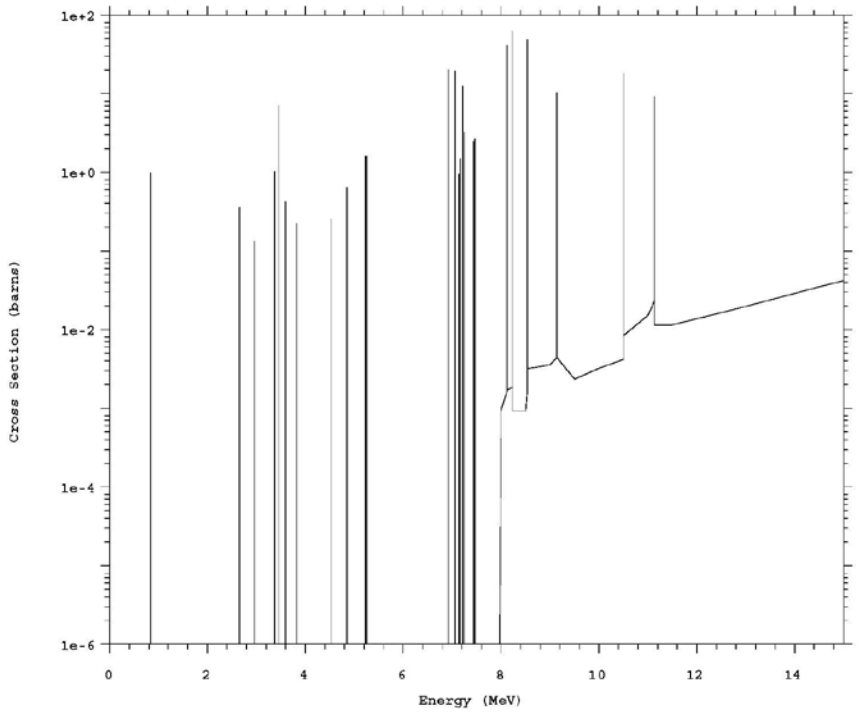


NRF resonances

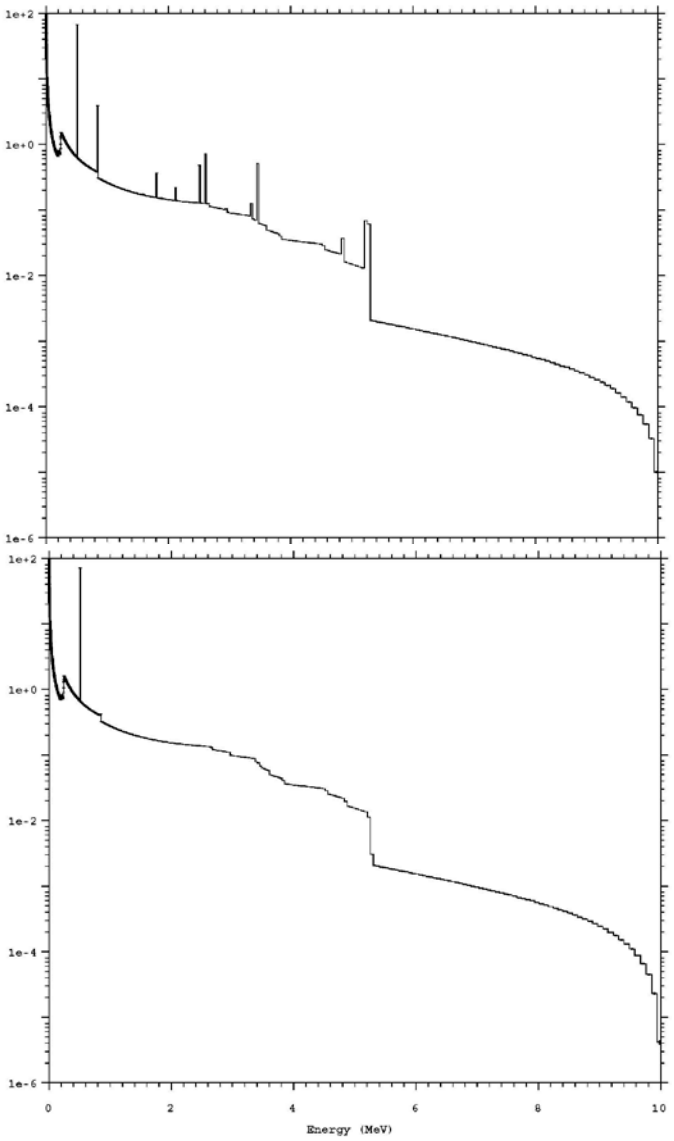


New NRF library (PN3-NRF) consists of 155 isotopes – data is undergoing verification and benchmarking

Fe-56

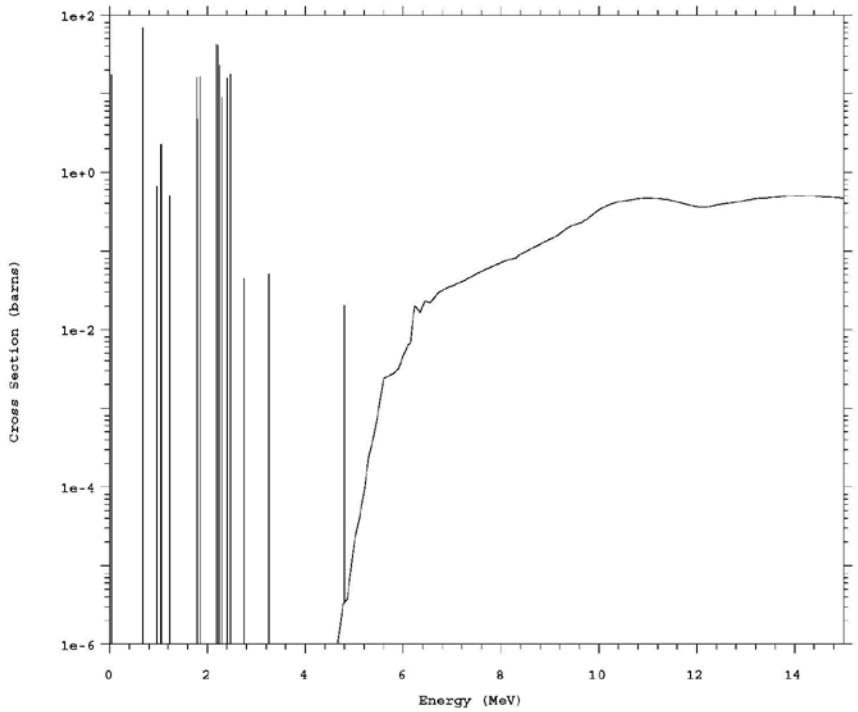


NRF resonances

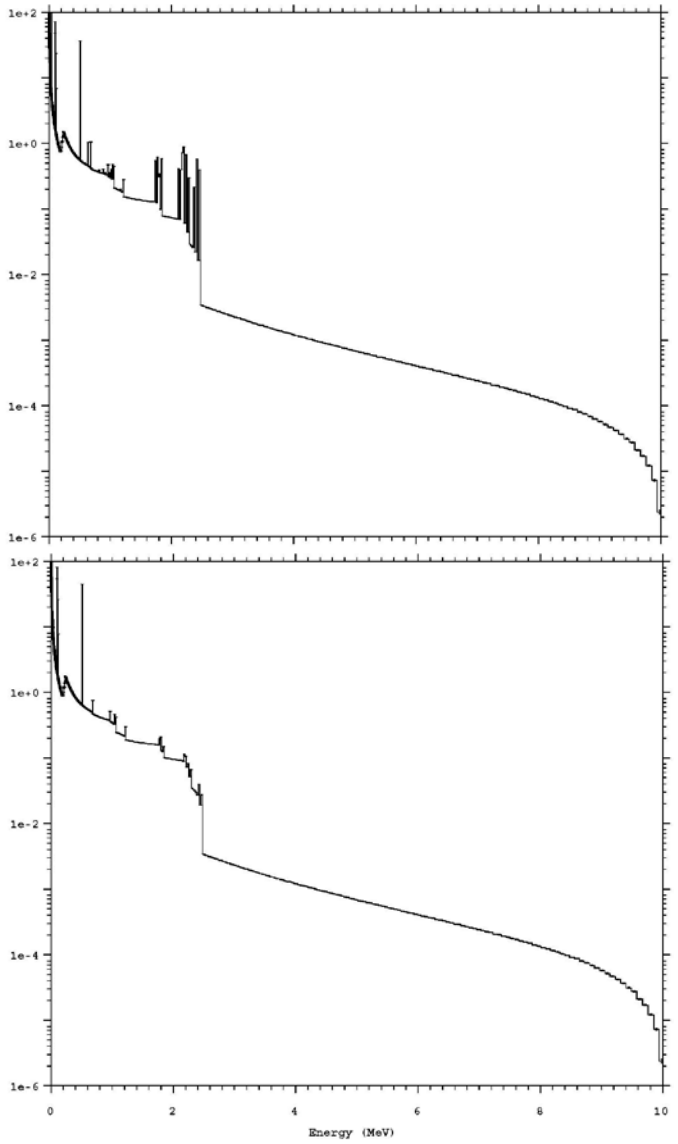


New NRF library (PN3-NRF) consists of 155 isotopes – data is undergoing verification and benchmarking

U-238



NRF resonances



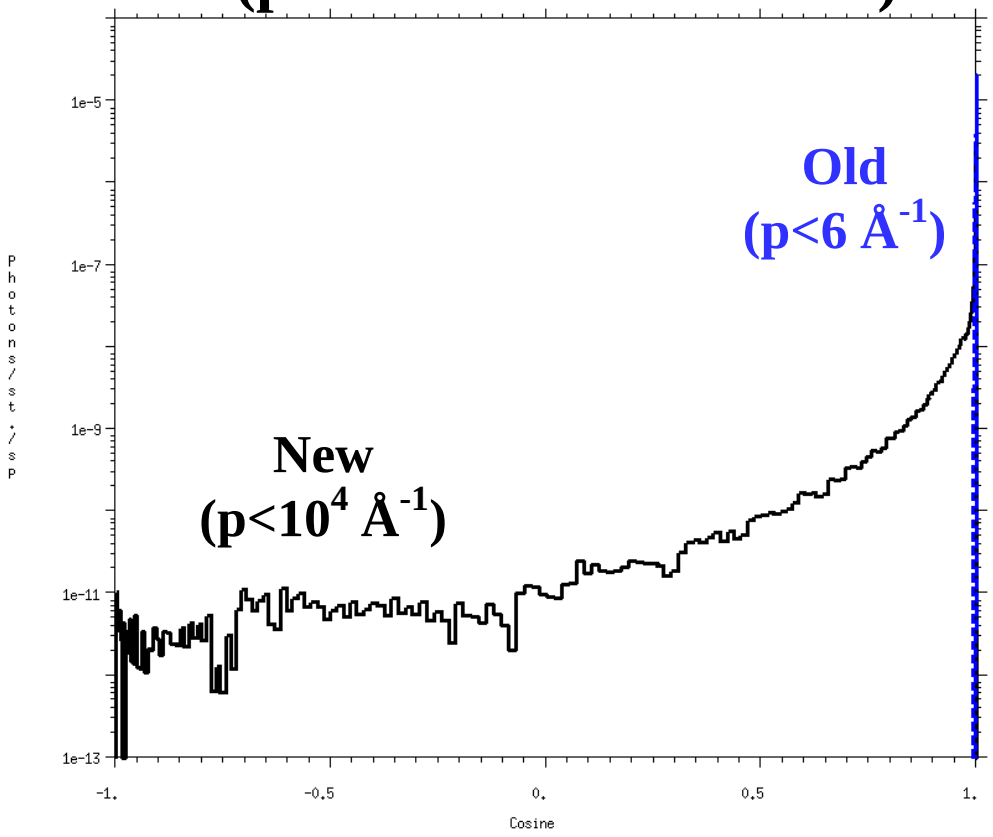
New NRF library (PN3-NRF) consists of 155 isotopes

```
6012.30u 11.896910 pn3-nrf 0 1 8705 21288
6013.30u 12.891650 pn3-nrf 0 1 14039 43407
7014.30u 13.882780 pn3-nrf 0 1 24903 87785
7015.30u 14.871250 pn3-nrf 0 1 46862 88074
8016.30u 15.853160 pn3-nrf 0 1 68893 63851
8017.30u 16.853100 pn3-nrf 0 1 84868 104839
8018.30u 17.844540 pn3-nrf 0 1 111090 131883
11023.30u 22.792280 pn3-nrf 0 1 144073 548759
12024.30u 23.779000 pn3-nrf 0 1 281275 96090
12025.30u 24.771200 pn3-nrf 0 1 305310 61418
12026.30u 25.759390 pn3-nrf 0 1 320677 91818
13027.30u 26.749750 pn3-nrf 0 1 343644 28931
14028.30u 27.737000 pn3-nrf 0 1 350889 59863
14029.30u 28.727560 pn3-nrf 0 1 365867 527876
14030.30u 29.716280 pn3-nrf 0 1 497848 144928
16032.30u 31.697410 pn3-nrf 0 1 534092 87570
16033.30u 32.688220 pn3-nrf 0 1 555997 492649
16034.30u 33.676060 pn3-nrf 0 1 679172 47782
16036.30u 35.658100 pn3-nrf 0 1 691130 82817
17035.30u 34.668450 pn3-nrf 0 1 711847 555680
17037.30u 36.648340 pn3-nrf 0 1 850779 589400
18036.30u 35.658560 pn3-nrf 0 1 998141 90231
18038.30u 37.636610 pn3-nrf 0 1 1020711 93149
18040.30u 39.619080 pn3-nrf 0 1 1044011 567232
...
```

Acknowledgements to:
Vladimir Mozin, LANL, N-4
Alton Coalter, Missouri-Columbia
Alex McKinney, LANL, D-5

Physics Enhancements – Form Factors

1.7 MeV photons into U
(p=momentum transfer)



Physics Enhancements – Delayed Gamma Algorithm Improvements

Case	Description	Execution Time	
		Multigroup	Line
1	15-MeV neutrons into ^{60}Ni	-99%	-99%
2	800-MeV protons into Cu	-98%	-86%
3	800-MeV protons into HEU	-97%	-88%

- **Use once-calculated CDFs for all multigroup residuals & prominent line-data residuals**
- **Analytic integration for simple decay**
- **Use of a threshold parameter to eliminate low-level lines**

Physics Enhancements – M & MX Card Enhancements

```
M & MX Card Enhancements
1  1  -1  -1  imp:n=1
2  0       1  imp:n=0

1 so 5

m0    nlib=.50c  hlib=.70h
m1     1001 2    1002 3e-4   8016  1
mx1:n  1001.60c     j        8016.70c
mode  n h
sdef
```

1. **m0: Load ENDF V neutron libraries (50c) and ENDF VII proton libraries (70h) by default.**
2. **m1: Define material (water).**
3. **mx1:n : Specify ENDF VI (60c) library for hydrogen and ENDVII (70c) for oxygen.**
4. **Can be used for proton and photonuclear libraries too.**

Physics Enhancements – M & MX Card Enhancements

```
    table    length

                        tables from file endf60

no particle-production data for ipt=  9 from   1001.60c
  1001.60c    1782  1-h-1 from endf-vi.1                                          mat 125      11/25/93

                        tables from file endf5p

no particle-production data for ipt=  9 from   1002.50c
  1002.50c    2447  njoy                                                      (  1302)      79/07/31.

                        tables from file endf70a

particle-production data for ipt=  9 being used from   8016.70c
particle-production data for ipt= 31 being expunged from   8016.70c
particle-production data for ipt= 32 being expunged from   8016.70c
particle-production data for ipt= 34 being expunged from   8016.70c
  8016.70c  186935   8-O - 16 at 293.6K from endf/b-vii.0 njoy99.248             mat 825      08/25/07

                        tables from file endf70prot

  1001.70h   15895  acer                                                         mat 125      09/17/07
  1002.70h    5962  acer                                                         mat 128      09/17/07
  8016.70h   54535  acer                                                         mat 825      09/17/07
```

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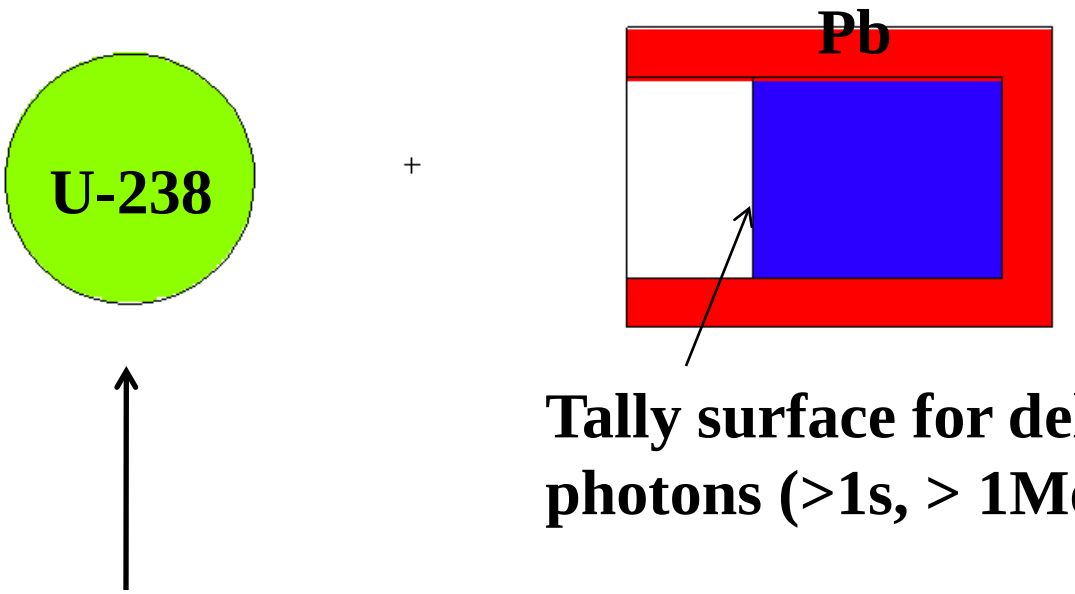
Tally Enhancements – FT ROC

```
Test FT ROC - Generate signal/noise PDFs - Pb shield
1   0           -1  2  7  5  imp:p=1
2   0           -2           imp:p=1
4   1 -5.16     -4           imp:p=1
5   2 -19.0     -5           imp:p=1
6   0           -6           imp:p=1
7   3 -11.3     -7  4  6     imp:p=1
8   0            1           imp:p=0

1 RPP  -100 100 -100 100 -100 100
2 SO   5.0
3 PZ   0.0
4 RCC  20 0 25 0 0 10 4.0
5 SPH  20 0  0 5.0
6 RCC  20 0 20 0 0  5 4.0
7 RCC  20 0 20 0 0 17 6.0

MODE p n
M1     32074.70c 1
M2     92238.70c 1
M3     82208.70c 1
MX2:P  model
CUT:N  60e8
CUT:P  60e8
PHYS:P j 1 j -1 j -101
SDEF PAR=P ERG=D1 X=FERG D2 Y=FERG D3 Z=FERG D4
TME=FERG D7
     VEC=1 0 0 DIR=FERG D8 CEL=1 WGT=1 $
1e7+200*200*6*10/3.7=10648648
SI1 S       5       6
SP1    0.9391  0.0609
c      SB1       1     1
DS2 S  15  16
DS3 S  25  26
DS4 S  35  36
DS7 S  45  46
DS8 S  55  56
```

```
c
SI15 L  5.1
SP15      1
SI25 L  0.0
SP25      1
SI35 L  0.0
SP35      1
c
SI16 -100 100
SP16    0   1
SI26 -100 100
SP26    0   1
SI36 -100 100
SP36    0   1
c
SI45 0 0.000010e8
SP45 0    1
SI46 0 60e8
SP46 0    1
c
SI55 L 1
SP55   1
SI56 -1 1
SP56  0 1
c
SI5 L 15.0
SP5      1
#    SI6        SP6
    1e-3         0
    1.00e+00     1
    10.00e+00    0.1
c
f4:p  2
f1:p  4.3
e1    1.0 100.0
t1    0.001e8 60e8
ft1   scx 1 roc 10648648
tf1   1 1 1 1 1 1 2 2   1 1 2 1 1 1 2 2
nps   1064864800
prdmp  j 106486480 1 2 10648648
```

Tally Enhancements – FT ROC

Background photon spectrum throughout

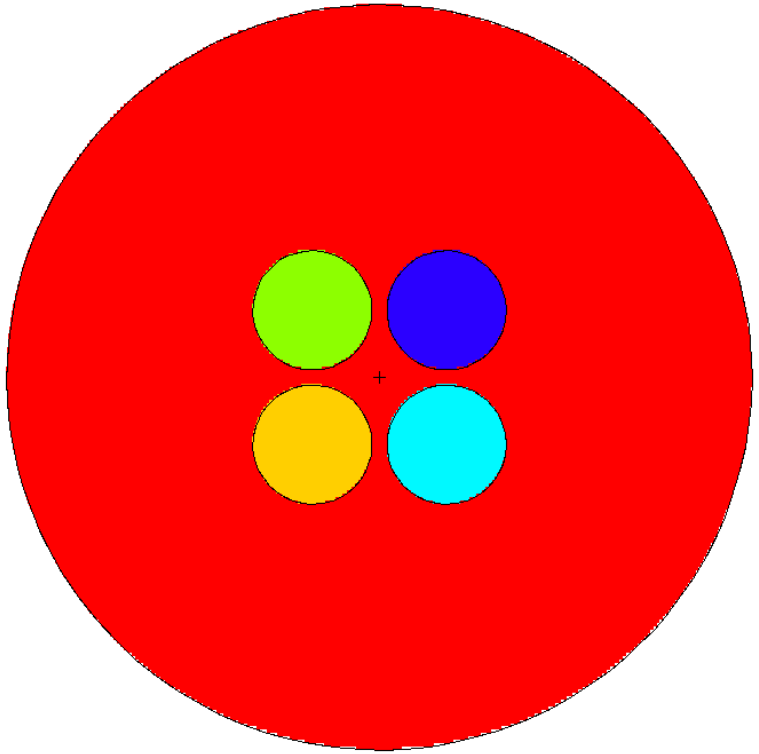


Tally Enhancements – FT ROC

```
1roc curve for tally   1   100 batches, signal mean= 1.488E+01 noise mean= 8.290E+00 nps =  1064864800  print table 163

  abscissa            ordinate                plot of probability of detection versus probability of false alarm - 0 to 100 percent
    noise               signal:--------10--------20--------30--------40--------50--------60--------70--------80--------90-------100
     1.000              12.000|         | x       |         |         |         |         |         |         |         |         |
     2.000              31.000|         |         |         |x        |         |         |         |         |         |         |
     3.000              47.000|         |         |         |         |      x  |         |         |         |         |         |
     4.000              56.000|         |         |         |         |         |     x   |         |         |         |         |
     5.000              56.000|         |         |         |         |         |     x   |         |         |         |         |
     6.000              65.000|         |         |         |         |         |         |    x    |         |         |         |
     7.000              65.000|         |         |         |         |         |         |    x    |         |         |         |
     8.000              71.000|         |         |         |         |         |         |         |x        |         |         |
     9.000              71.000|         |         |         |         |         |         |         |x        |         |         |
    10.000              71.000|         |         |         |         |         |         |         |x        |         |         |
    11.000              77.000|         |         |         |         |         |         |         |      x  |         |         |
    12.000              79.000|         |         |         |         |         |         |         |        x|         |         |
    13.000              79.000|         |         |         |         |         |         |         |        x|         |         |
    14.000              79.000|         |         |         |         |         |         |         |        x|         |         |
    15.000              79.000|         |         |         |         |         |         |         |        x|         |         |
    16.000              89.000|         |         |         |         |         |         |         |         |        x|         |
    17.000              89.000|         |         |         |         |         |         |         |         |        x|         |
    18.000              89.000|         |         |         |         |         |         |         |         |        x|         |
    19.000              89.000|         |         |         |         |         |         |         |         |        x|         |
    20.000              89.000|         |         |         |         |         |         |         |         |        x|         |
    21.000              91.000|         |         |         |         |         |         |         |         |         |x        |
    22.000              91.000|         |         |         |         |         |         |         |         |         |x        |
    23.000              91.000|         |         |         |         |         |         |         |         |         |x        |
    24.000              91.000|         |         |         |         |         |         |         |         |         |x        |
    25.000              91.000|         |         |         |         |         |         |         |         |         |x        |
    26.000              91.000|         |         |         |         |         |         |         |         |         |x        |
    27.000              91.000|         |         |         |         |         |         |         |         |         |x        |
    28.000              91.000|         |         |         |         |         |         |         |         |         |x        |
    29.000              91.000|         |         |         |         |         |         |         |         |         |x        |

cont. . .
```

Tally Enhancements – FTR RES Upgrade

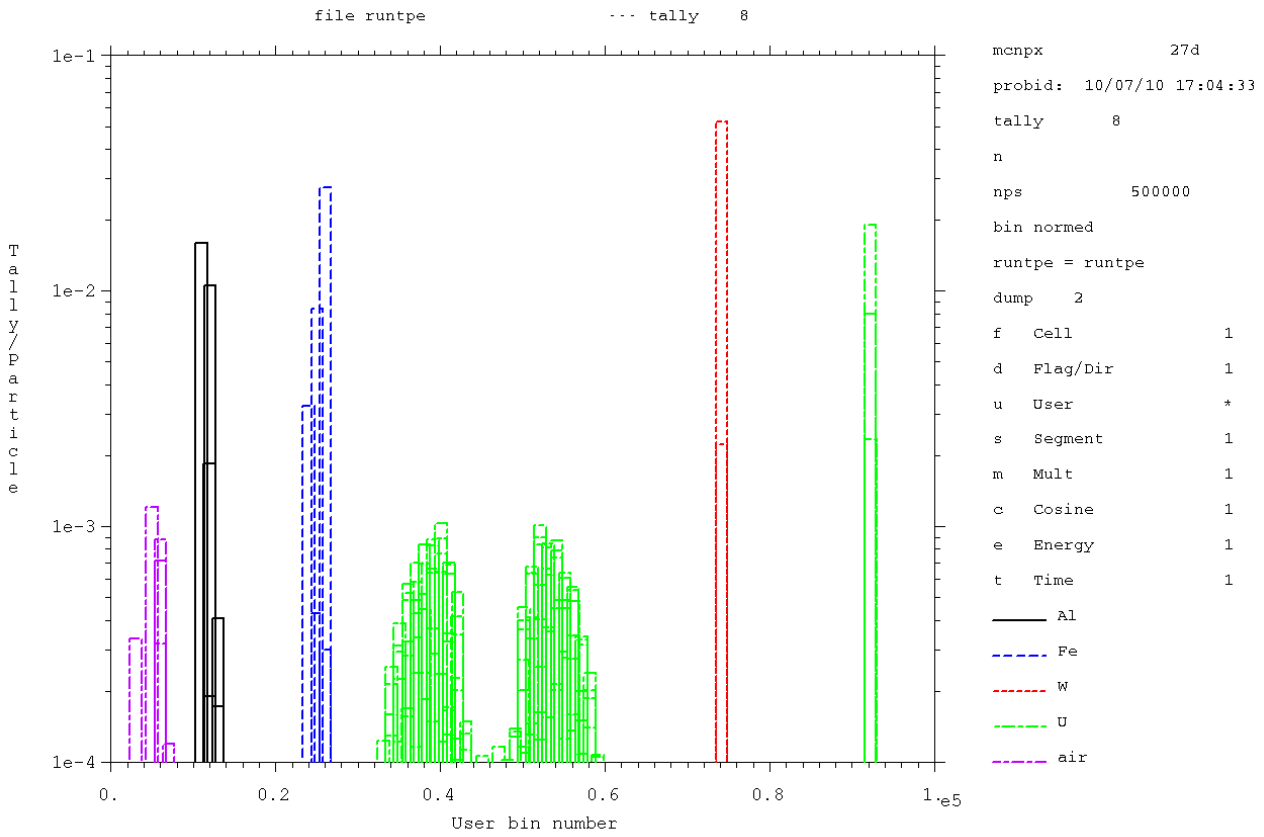
```
Test FT RES upgrades
1  1  -5    -1   imp:n=1
2  2  -5    -2   imp:n=1
3  3  -5    -3   imp:n=1
4  4  -5    -4   imp:n=1
5  5  -1e-2 -5 #1 #2 #3 #4 imp:n=1
6  0         5   imp:n=0

1  rcc  9  9 -10  0 0 20 8
2  rcc  9 -9 -10  0 0 20 8
3  rcc -9  9 -10  0 0 20 8
4  rcc -9 -9 -10  0 0 20 8
5  so 50

m1  13027  1           $ aluminum
m2  26056  1           $ iron
m3  74182  1           $ tungsten
m4  92238  1           $ uranium
m5  7014 0.8 8016 0.2  $ air
sdef
f8:n 1 2 3 4 5
ft8 res
nps 500000
prdmp 2j 1
```



14 MeV neutron source at center

Tally Enhancements – FT RES Upgrade

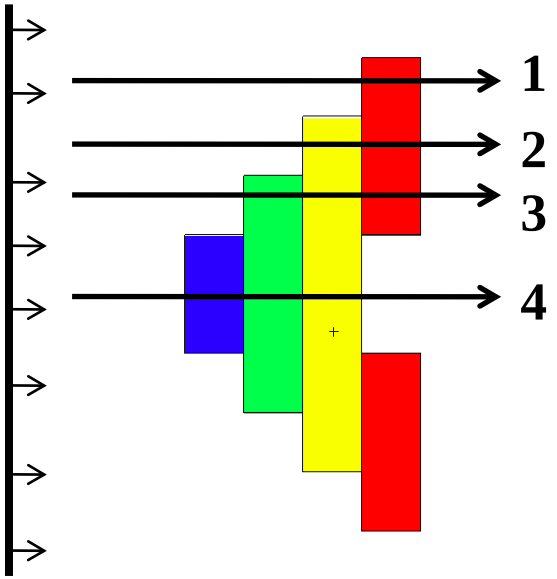
- **Coplot of cell bins showing different residual yields.**



Tally Enhancements – 4-Fold FT PHL

```
Test problem for 4-fold FT PHL
1 1 -1  -1 11 -12   imp:n=1
2 2 -1  -2 12 -13   imp:n=1
3 3 -1  -3 13 -14   imp:n=1
4 4 -1  -4 14 -15 1 imp:n=1
98 0   -99 #1 #2 #3 #4 imp:n=1
99 0    99             imp:n=0

1 cz 1
2 cz 2
3 cz 3
4 cz 4
11 pz 0
12 pz 1
13 pz 2
14 pz 3
15 pz 4
99 so 100

sdef par=| erg=200 vec=0 0 1
     axs=0 0 1 dir=1 rad=d1 pos 0 0 -1
si1 0 5
sp1 -21 1
m1 1001 2 8016 1
m2 26056 1
m3 13027 1
m4 74184 1
```

```
print
mode |
phys:| 200
nps 50
f16:| 1
f26:| 2
f36:| 3
f46:| 4
f8:n 1
ft8 PHL 1 16 1 1 26 1 1 36 1 1 46 1
e8  0 20 NT
fu8 0 20 NT
c8  0 20 NT
fs8 0 20 NT
fq8 s c e u
```



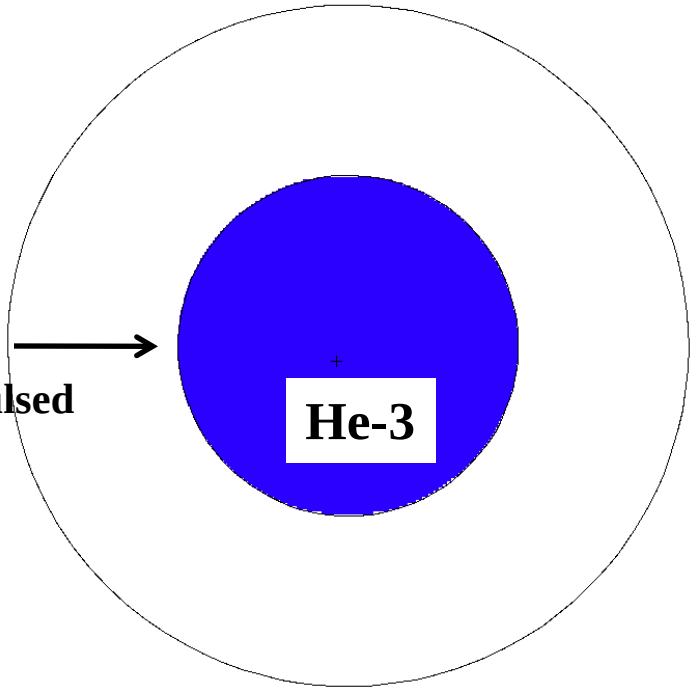
Tally Enhancements – 4-Fold FT PHL

- **Results reported as x^n bins where x is number of energy bins and n is the number of coincidence regions.**
- **This example: 4 regions with 2 energy bins (scored/not scored) produces 2^4 or 16 possible outcome bins.**
- **Scores marked in red show results of 4 possible outcomes.**

```
1tally   8        nps =       50
           tally type 8    pulse height distribution
           particle(s): neutron
           this tally is modified by   ft  phl

 cell  1
 segment bin:  -i           to  0.00000E+00
 cosine bin:  -1.           to  0.00000E+00
     user bin:       0.0000E+00           2.0000E+01
      energy
    0.0000E+00   0.00000E+00 0.0000   0.00000E+00 0.0000
    2.0000E+01   0.00000E+00 0.0000   0.00000E+00 0.0000

 cell  1
 segment bin:  -i           to  0.00000E+00
 cosine bin:   0.00000E+00 to  2.00000E+01
     user bin:       0.0000E+00           2.0000E+01
      energy
    0.0000E+00   0.00000E+00 0.0000   0.00000E+00 0.0000
    2.0000E+01   0.00000E+00 0.0000   6.00000E-02 0.5598

 cell  1
 segment bin:   0.00000E+00 to  2.00000E+01
 cosine bin:  -1.           to  0.00000E+00
     user bin:       0.0000E+00           2.0000E+01
      energy
    0.0000E+00   2.60000E-01 0.2386   0.00000E+00 0.0000
    2.0000E+01   0.00000E+00 0.0000   0.00000E+00 0.0000

 cell  1
 segment bin:   0.00000E+00 to  2.00000E+01
 cosine bin:   0.00000E+00 to  2.00000E+01
     user bin:       0.0000E+00           2.0000E+01
      energy
    0.0000E+00   1.80000E-01 0.3018   1.20000E-01 0.3830
    2.0000E+01   0.00000E+00 0.0000   0.00000E+00 0.0000
```

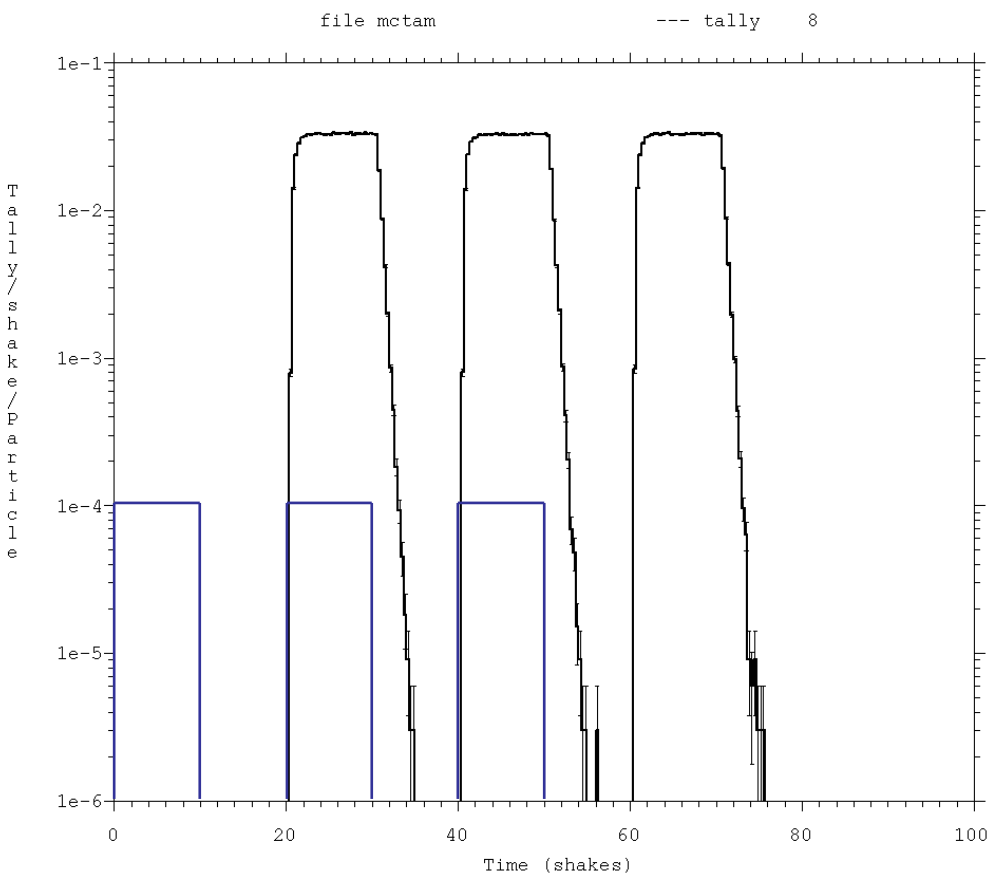
Tally Enhancements – Time Dep. FT PHL

```
Test Time dependent PHL Tally
1  1  -1   -1  imp:n=1
2  0     1 -2  imp:n=1
3  0        2  imp:n=0

1 so 10
2 so 20

m1  2003 1
mode n h p d t s a
nps 100000
phys:n 6j 2
cut:t j 1e-3
cut:h j 1e-3
cut:n j j 0 0
prdmp  5000 5000 1
sdef tme=d1 erg=1e-3  pos 0 0 -19 vec 0 0 1 dir
si1  0  10   20   30   40   50
sp1  0   1    0    1    0    1
f6:t  1
f16:h  1
f8:n 1
ft8 phl  2 6 1 16 1 0
t8 0 299i 100
```



Tally Enhancements – Time Dep. FT PHL

- **Blue curves show pulsed neutron source, black curves are He-3 detector response.**
- **Neutron flight time delay and spread in capture and ion energy deposition.**
- **1 shake = 10^{-8} s**



Test suite enhancements – versions 2.7.A, 2.7.B, 2.7.C, 2.7.D

Physics Enhancements

CEM upgrade to 03.02
Adjustable stopping-power grid
LLNL photofission multiplicities
Delayed gamma exact sampling
LLNL neutron fission multiplicities
Muonic x-ray enhancements
Delayed neutron spectra
NRF data in ACE libraries
Improved photoatomic form factors
DG algorithm improvements
M & MX card enhancements

Source Enhancements

Burnup enhancements
Pulsed sources
Beam source options

Tally Enhancements

Tally tagging
LET tally option
Quality factor tally option
Cyclic tally binning
ROC curve tally option
Residual tally upgrades
Triple & quadruple coincidences
Time-dependent pulse-height tallies

Variance Reduction Enhancements

Other Enhancements

MCPLOT graphics enhancements
Activation options (ACT card)
MCPLOT tally manipulations
Nested READ cards
Feature-based memory reduction

Other Enhancements – Nested READs

```
Test Nested Read option
1  1  -1  -1 imp:n=1
2  0       1 imp:n=01

1 so 5
```

File: data

```
read file=data  <----  read file=m1  <----
                       phys:n 20
                       sdef
```

File: m1

```
m1  1001 2 8016 1
```

```
    1-       test Nested Read option
    2-       1  1  -1  -1 imp:n=1
    3-       2  0       1 imp:n=01
    4-
    5-       1 so 5
    6-
    7-       read file=data
****************************** begin read ************************************
    8-       read file=m1
****************************** begin read ************************************
    9-       m1  1001 2 8016 1
****************************** end read **************************************
   10-       phys:n 20
   11-       sdef
```

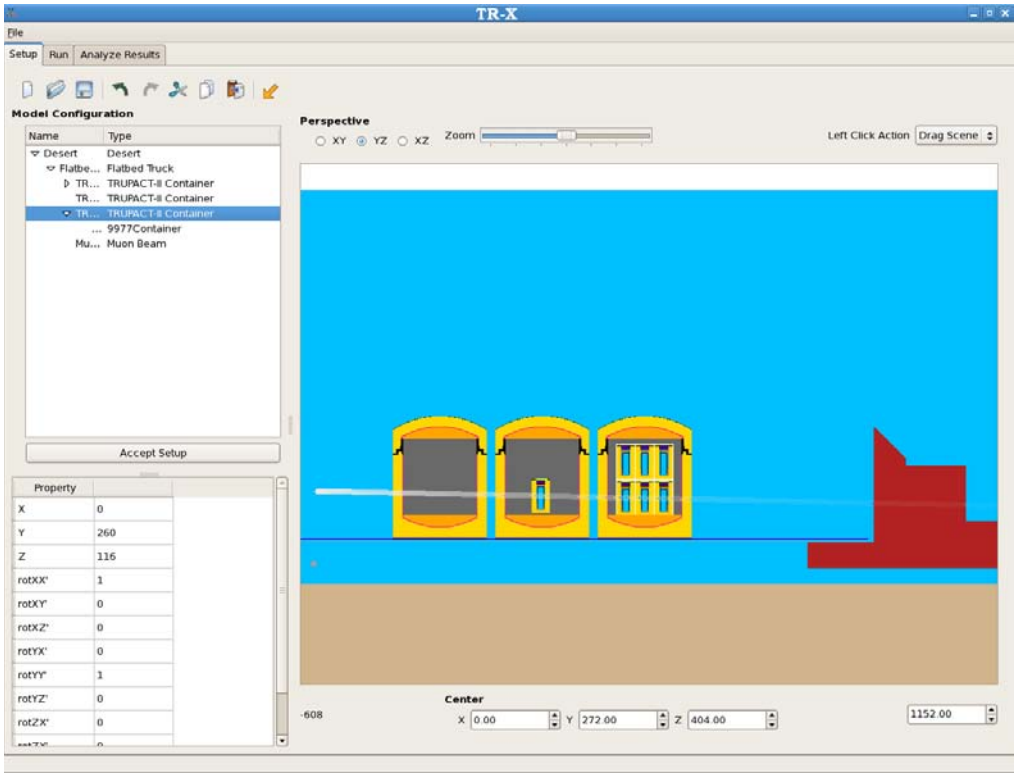
Other Enhancements – ACT Card

```
Test new act card functions
1  1  -10  -1 imp:n=1
2  0        1 imp:n=0

1 so 1

sdef
mode n p
m1 1001 6 92235 1
f4:p 1
e4 0 999i 10
t4 1e4 9ilog 1e11
f14:n 1
e14  0 99i 10
t14 1e4 9ilog 1e11
act fission=all nonfiss=all dn=both dg=mg thresh=0.95
```

Keywords on ACT card replace PHYS card numeric entries

TR-X Graphical Interface

- Object (e.g. truck, car) based simulation wrapper for MCNPX
- Compose Scenes from prebuilt objects, Wizards help configure physics etc.
- Runtime submission agent for local or cluster jobs.
- Tally and output parser for analysis
- Enhanced Error checking
- Runs or PC/Mac/Linux



Summary

- MCNPX 2.7.D was released to Beta Users Oct 1, 2010.
  - Extensions document LA-UR-10-07031.
- MCNPX 2.7.0 scheduled for release to RSICC ~Jan 2010
- Follow-on development will be in MCNP6 (merged MCNPX & MCNP5).

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