LA-UR-09-2026

Physics and Algorithm Enhancements for a Validated MCNPX Monte Carlo Simulation Tool

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DNDO/NSF ARI Grantees Conference

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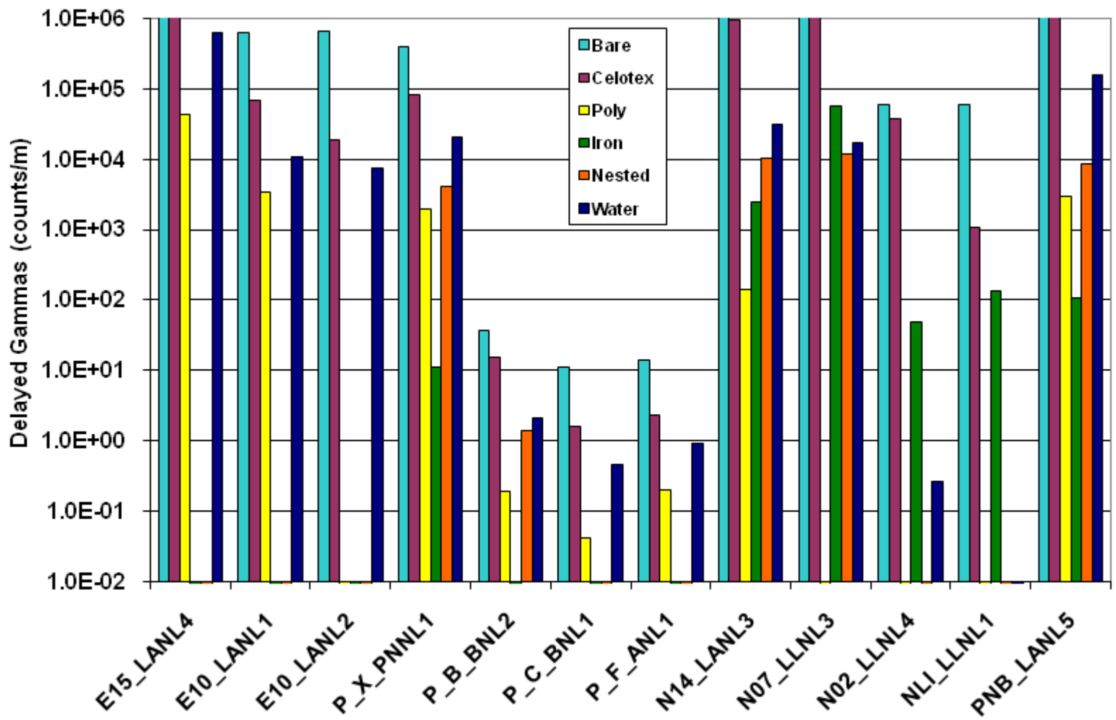
Outline

- MCNPX overview
- DNDO MCNPX project overview
- Highlights of various features

Simulation status as of June 2006:
- Results had large uncertainties
- Execution times were very long
- Lacked background contributions
- One-off delayed gamma treatment



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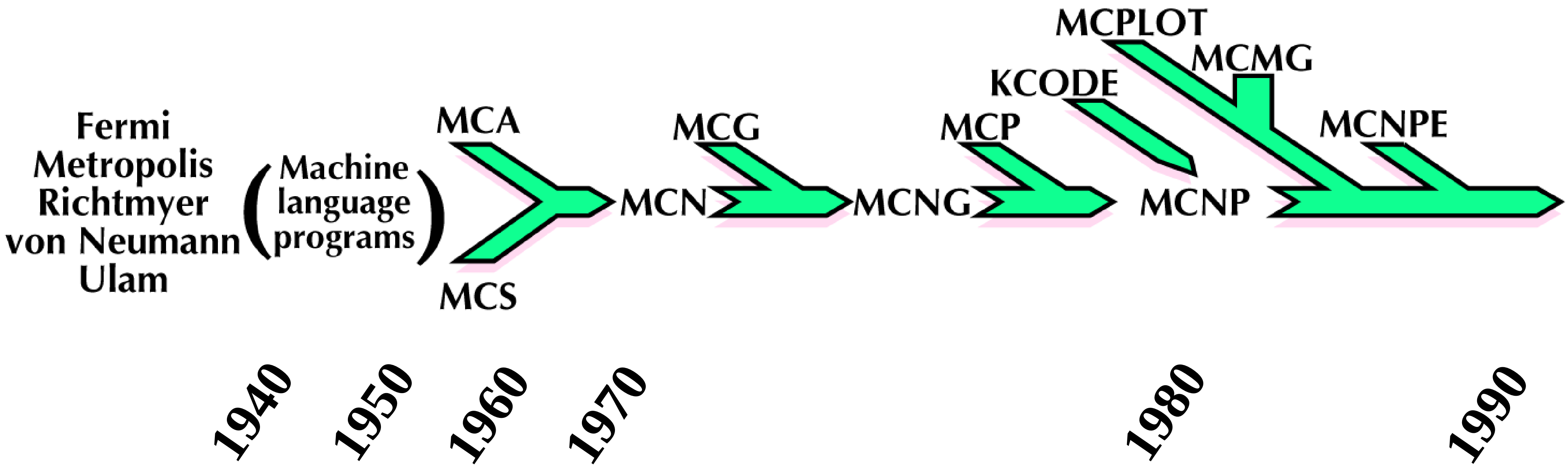
MCNPX is a 3-D, all-particle, all-energy Monte Carlo transport code

- **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)

The previous century of development – it wasn't always called "MCNP"



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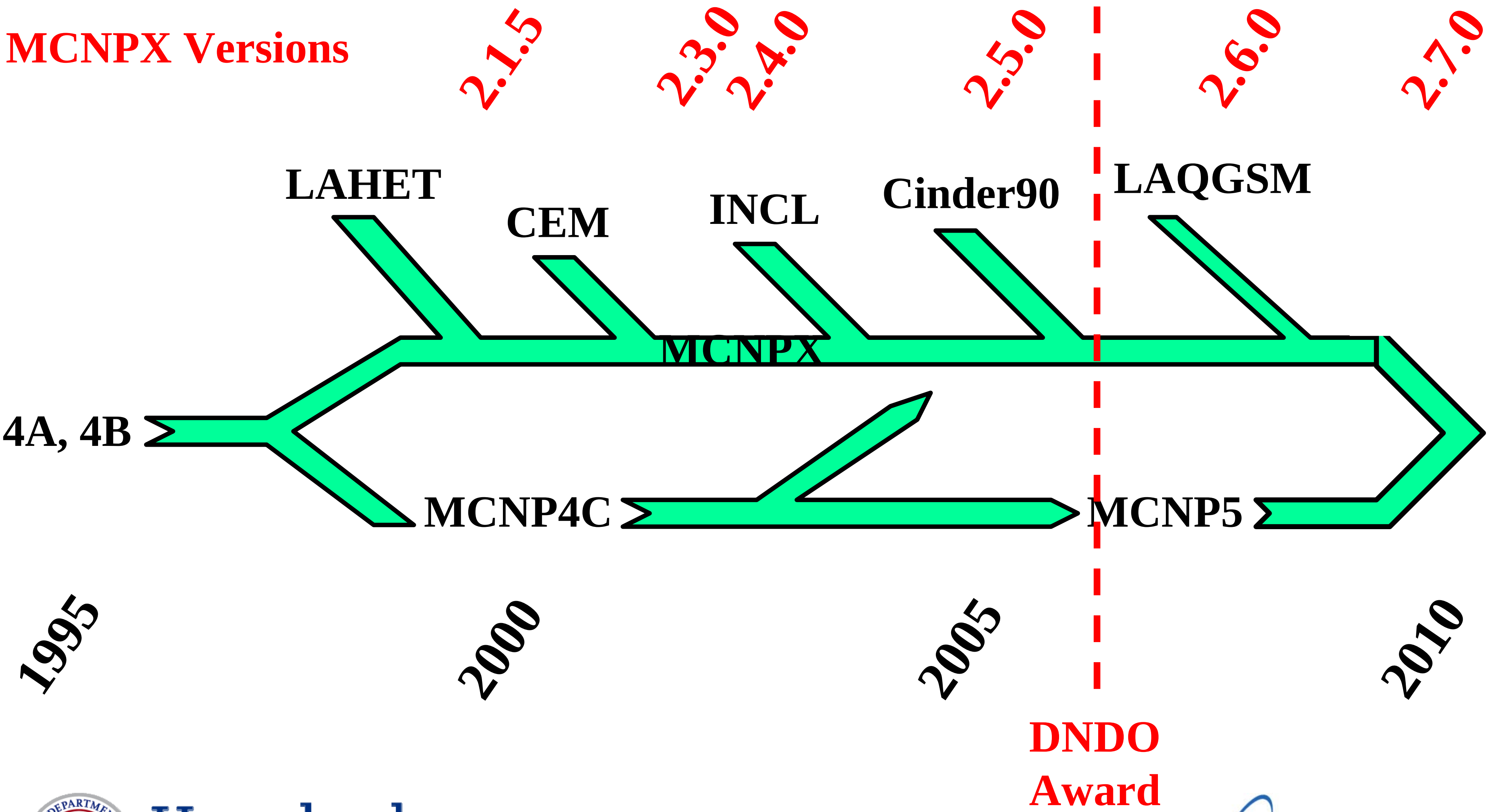
The current century of development – why the split into MCNP and MCNPX?



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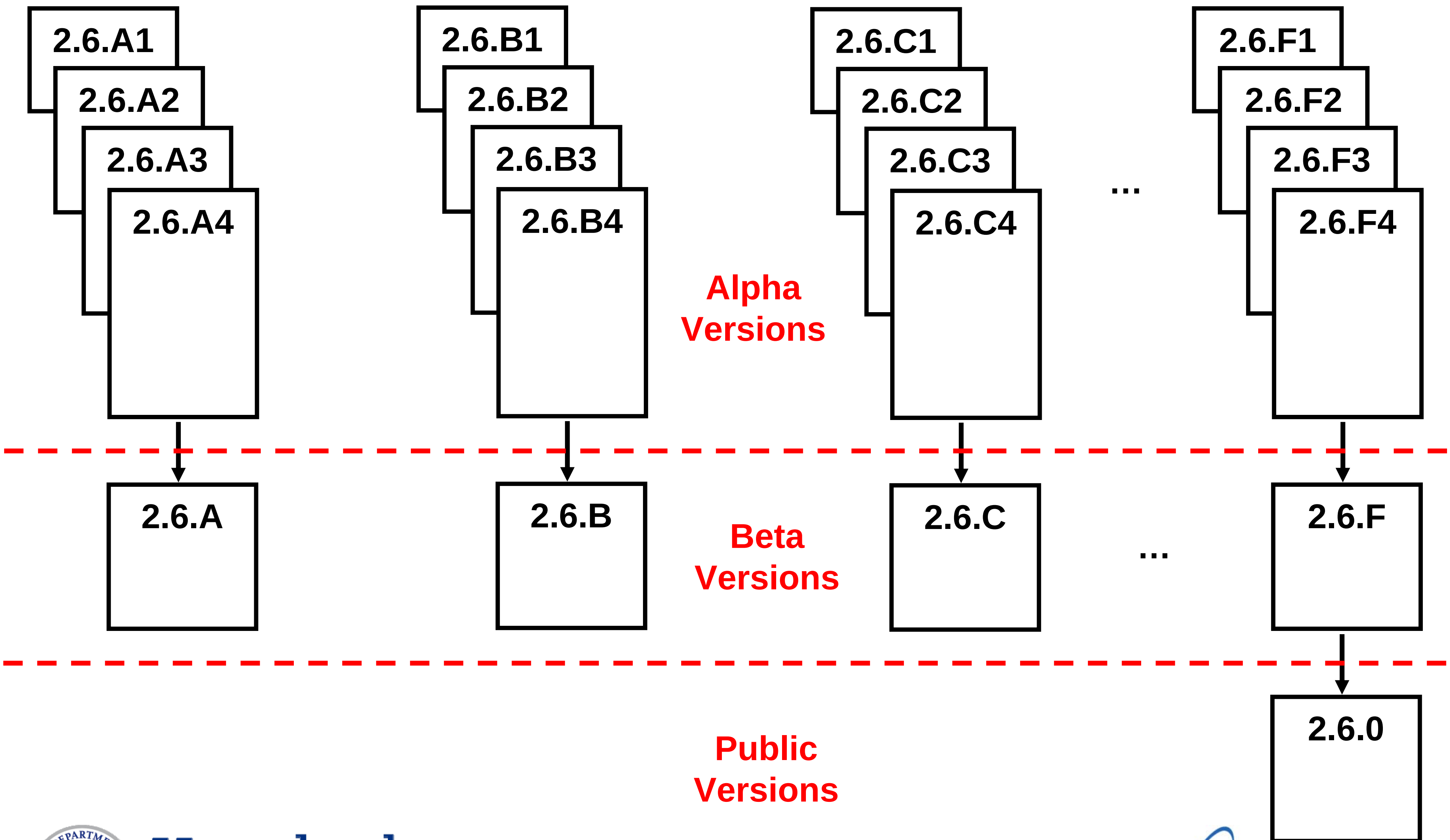
The current century of development – why so many versions of MCNPX?



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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

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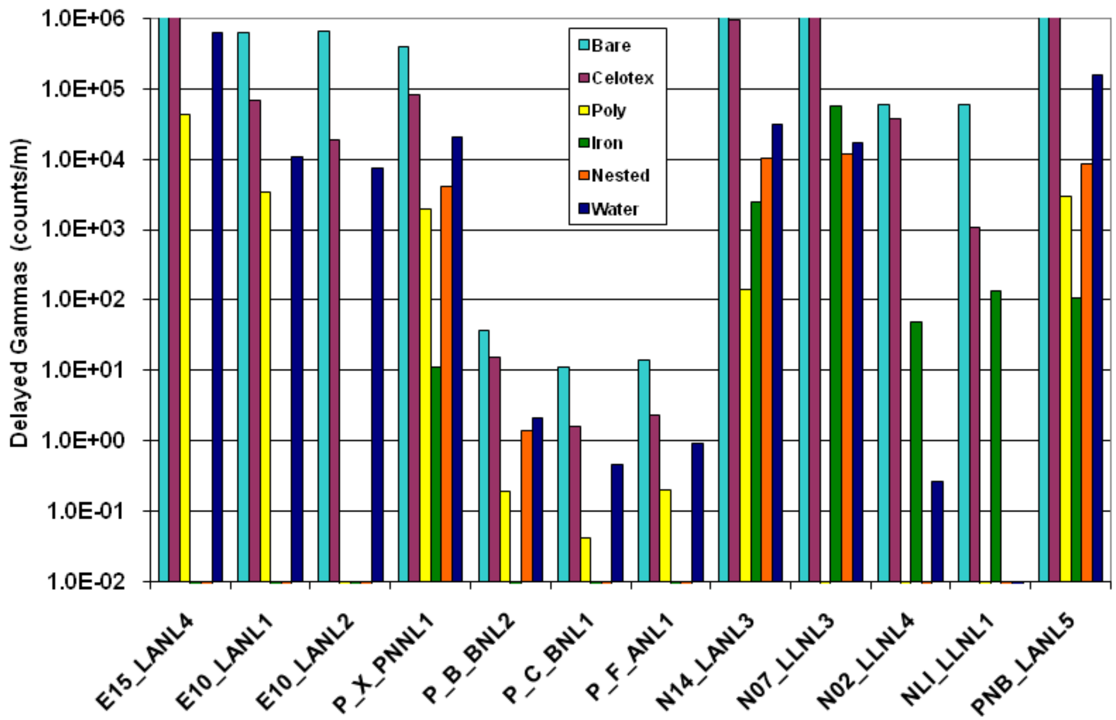

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MCNPX is an essential tool for predicting radiation detector system performance

- U.S. needs a single end-to-end (i.e., source-to-detector) simulation tool to evaluate, design, and optimize SNM detection systems
- Physics and algorithm upgrades were identified to enable simulation of DHS detection systems
- Upgrades for the MCNPX transport code are being developed to:
  - Incorporate all signal and background signatures
  - Span the range of DHS design and analysis needs
  - Predict and optimize receiver-operator characteristic (ROC) curves

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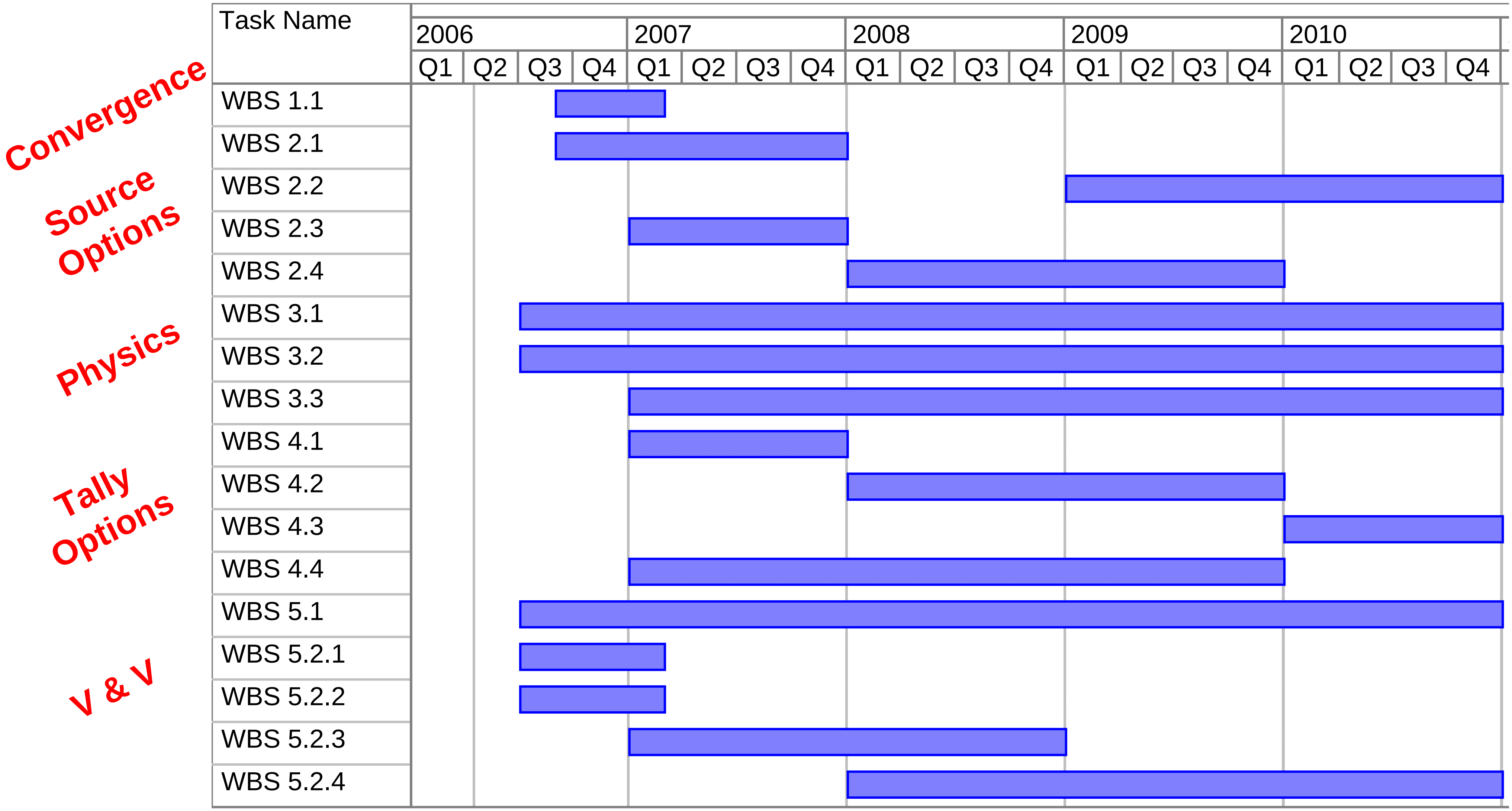
Project plan includes a prioritized approach with a commitment to verification and validation

- Created a prioritized list of capabilities to address gaps
  - Includes ~12 features implemented over 5 years
  - Important physics upgrades developed first
  - Algorithm and data refinements primarily in the out years
- Accomplish objectives by:
  - Following standard SQA procedures (verification)
  - ~~Validating new physics with benchmark measurements~~ Postponed
  - Releasing new MCNPX versions to DHS users
- Project contributors
  - MCNPX code development team (X-3, D-5)
  - Nuclear data and modeling team (T-16)
  - ~~Advanced nuclear technology group (N-2)~~ Postponed

Project Gantt chart – top level tasks separated into five categories



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Plans and Schedule – Top level FY06 tasks

- Automatic production of background activation (1 of 5 yr)
- Spherical weight-windows for enhanced convergence (1 yr)
- Automatic production of radioactive sources (1 of 2 yr)
- Test suite improvements to provide verification (1 of 5 yr)
- Development of a benchmark plan for validation (1 yr)
- Improvements in photonuclear data (1 of 5 yr)
- Experimental work authorizations for FY07 tasks (1 yr)

Plans and Schedule – Top level FY07 tasks

- Automatic production of background activation (2 of 5 yr)
- Display of spherical mesh tally data (1 yr)
- Automatic production of radioactive sources (2 of 2 yr)
- Test suite improvements to provide verification (2 of 5 yr)
- Correlated secondary particle production (1 of 4 yr)
- Improvements in photonuclear data (2 of 5 yr)
- Segregation of tallies into signal and noise (1 of 3 yr)
- Incorporation of muon capture and NRF physics (1 of 2 yr)

Plans and Schedule – Top level FY08 tasks

- Automatic production of background activation (3 of 5 yr)
- Pulsed sources (1 of 2 yr)
- Natural background sources (1 of 2 yr)
- Test suite improvements to provide verification (3 of 5 yr)
- Correlated secondary particle production (2 of 4 yr)
- Improvements in photonuclear data (3 of 5 yr)
- Segregation of tallies into signal and noise (2 of 3 yr)
- Incorporation of muon capture and NRF physics (2 of 2 yr)
- Standard detector responses (1 of 2 yr)

Plans and Schedule – Top level FY09 tasks

- Automatic production of background activation (4 of 5 yr)
- Pulsed sources (2 of 2 yr)
- Natural background sources (2 of 2 yr)
- Test suite improvements to provide verification (4 of 5 yr)
- Correlated secondary particle production (3 of 4 yr)
- Improvements in photonuclear data (4 of 5 yr)
- Segregation of tallies into signal and noise (3 of 3 yr)
- Incorporation of muon capture and NRF physics (2 of 2 yr)
- Standard detector responses (2 of 2 yr)

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Code releases over the last 3 years, with DNDO features highlighted in red

Version 2.6.A	December, 2005
Transmutation, Long file names, STOP card	
Version 2.6.B **DNDO Award** →	June, 2006
CEM 03, new PHTLIB, predictor-corrector for burnup	
Version 2.6.C	December, 2006
Spherical weight windows, delayed particle production	
Version 2.6.D	June, 2007
Coupled energy-time weight windows, activation	
Version 2.6.E	November, 2007
Heavy-ion transport, muon capture physics, photofission yields	
Version 2.6.F	March, 2008
Spontaneous photons, dynamic material burnup	
Version 2.6.0	**April, 2008**
Version 2.7.A	November, 2008
Pulsed sources, tally tagging, MCPLOT enhancements	
Version 2.7.B	April, 2009
LLNL photofission multiplicities, LET tally, CEM upgrade	
Version 2.7.C	July, 2009
DG exact sampling, ACT card, MCPLOT manipulations	

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MCNPX public version 2.5.0 – prior to DNDO award

Physics Enhancements

Mix & match of libraries and models
CEM upgrade to 2K
INCL 4 & ABLA physics models
Secondary-particle production
Neutron fission multiplicity
S(a,b) secondary-energy smoothing
Photonuclear physics model
Photon Doppler broadening

Source Enhancements

Positron sources
Spontaneous fission sources
Multiple source particles
Default VEC for cylindrical sources
Extension of the TR keyword

Tally Enhancements

Lattice tally speedup
Anticoincidence pulse-height tally
Coincidence capture pulse-height tally
Residual nuclei pulse-height tally

Variance Reduction Enhancements

WWG superimposed mesh plots
Variance reduction with pulse-height tallies

Other Enhancements

Lattice index labeling
Color contour and mesh tally plots
READ card
HISTP card extension
EXTRAN/detector underflow control
8-byte integers
Parallel processing with MPI

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MCNPX public version 2.6.0 – DNDO sponsored features account for ~50% of new capabilities

Physics Enhancements

Muon capture physics
Integration of the LAQGSM event generator
Heavy-ion transport
Integration of the Cinder code
Photo-fission yield data

Delayed particles from activation
Upgrade of the CEM event generator
Ion production from library neutron capture
Gravity effects for neutrons
Updated photon de-excitation data

Source Enhancements

Transmutation with KCODE
Acceleration of KCODE source convergence
Spontaneous decay photon sources

Tally Enhancements

Termination based on precision
Spherical mesh tally plots
Differential tallies extended to library events

Variance Reduction Enhancements

Spherical mesh WW (weight windows)
Coupled space-energy-time WW
Additional WW controls

Other Enhancements

Long file names
Proton step size control
Output for induced-fission multiplicity
Several graphics enhancements

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MCNPX public version 2.7.0 – DNDO sponsored features account for ~70% of new capabilities

Physics Enhancements

Delayed gamma exact sampling
CEM upgrade to 03.02
LLNL photofission multiplicities
LLNL neutron fission multiplicities
Muonic x-ray enhancements
Delayed neutron spectra
NRF data in ACE libraries
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Source Enhancements

Pulsed sources
Beam source options
Natural background sources

Tally Enhancements

Tally tagging
LET tally option
Quality factor tally option
Cyclic tally binning

Variance Reduction Enhancements

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Other Enhancements

MCPLOT graphics enhancements
MCPLOT tally manipulations
Activation options (ACT card)

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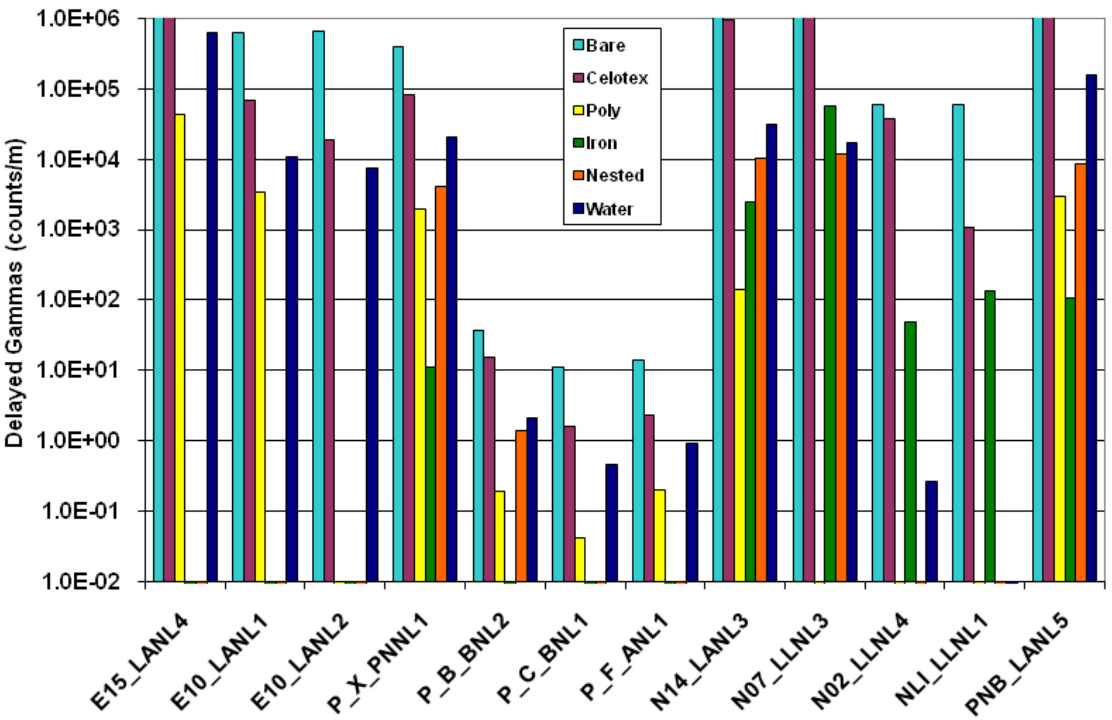
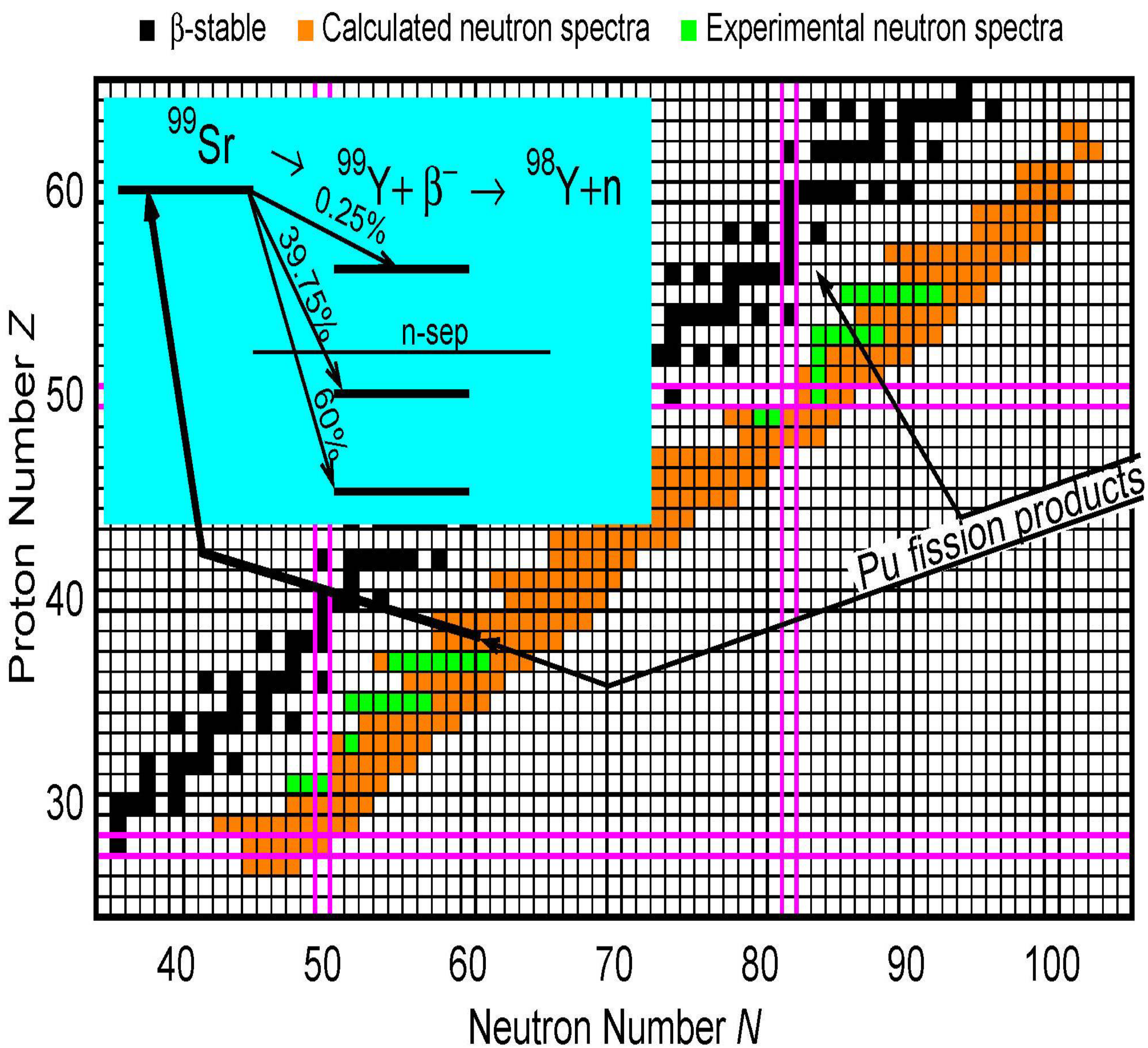


Delayed neutron (DN) spectra have been calculated for important fission precursors



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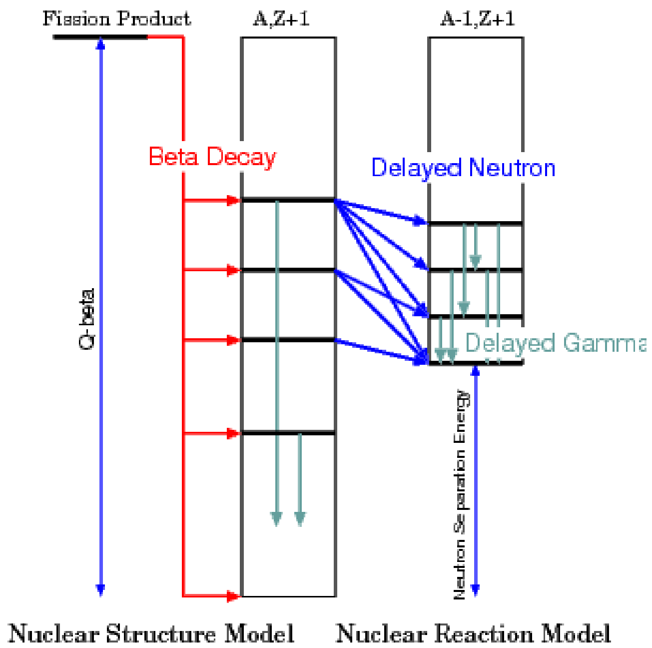
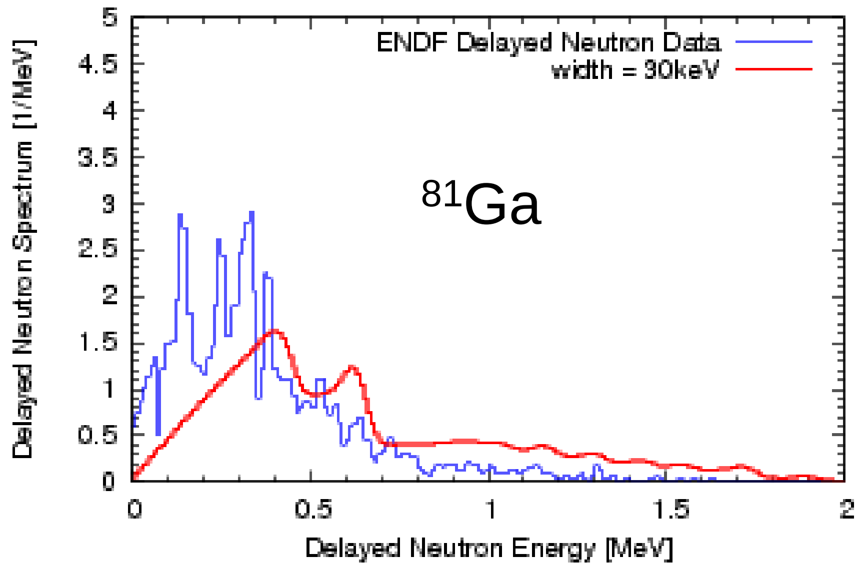
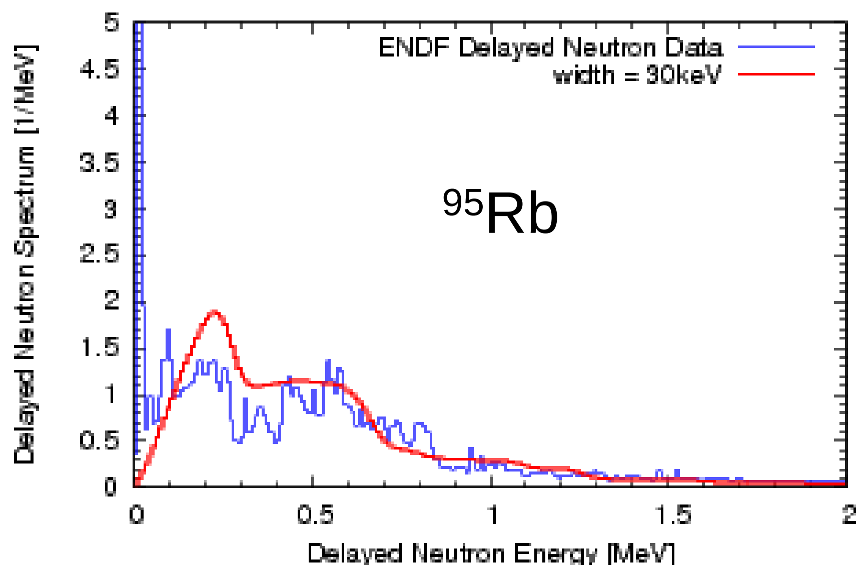




34 of the 270 ENDF DN precursors are based on measured data, while the others use simple functions. We have updated these data based on a LANL nuclear structure model and a statistical Hauser-Feshbach model.



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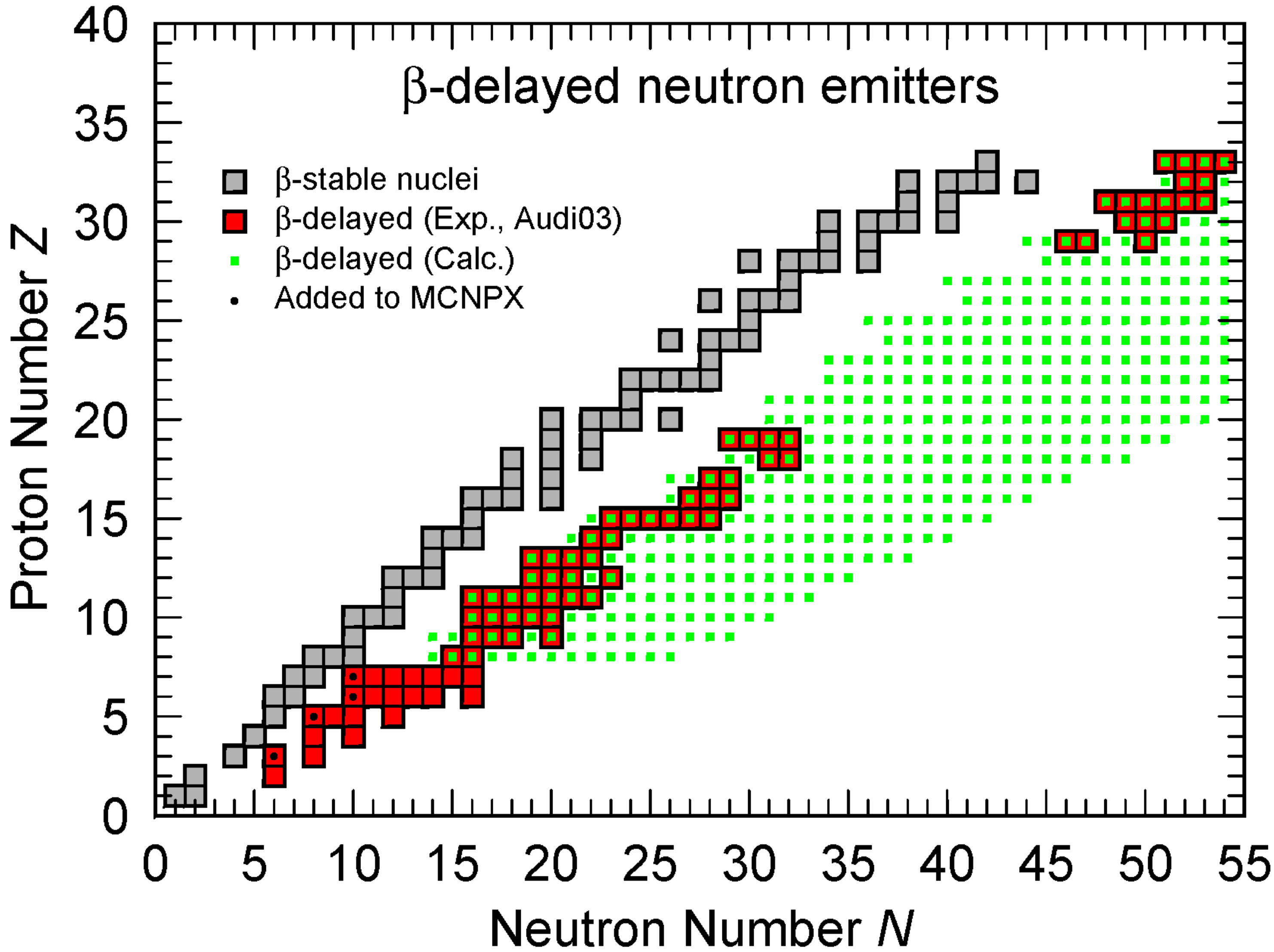
Delayed neutron spectra have also been calculated for lighter isotopes – measured data used for Z<8



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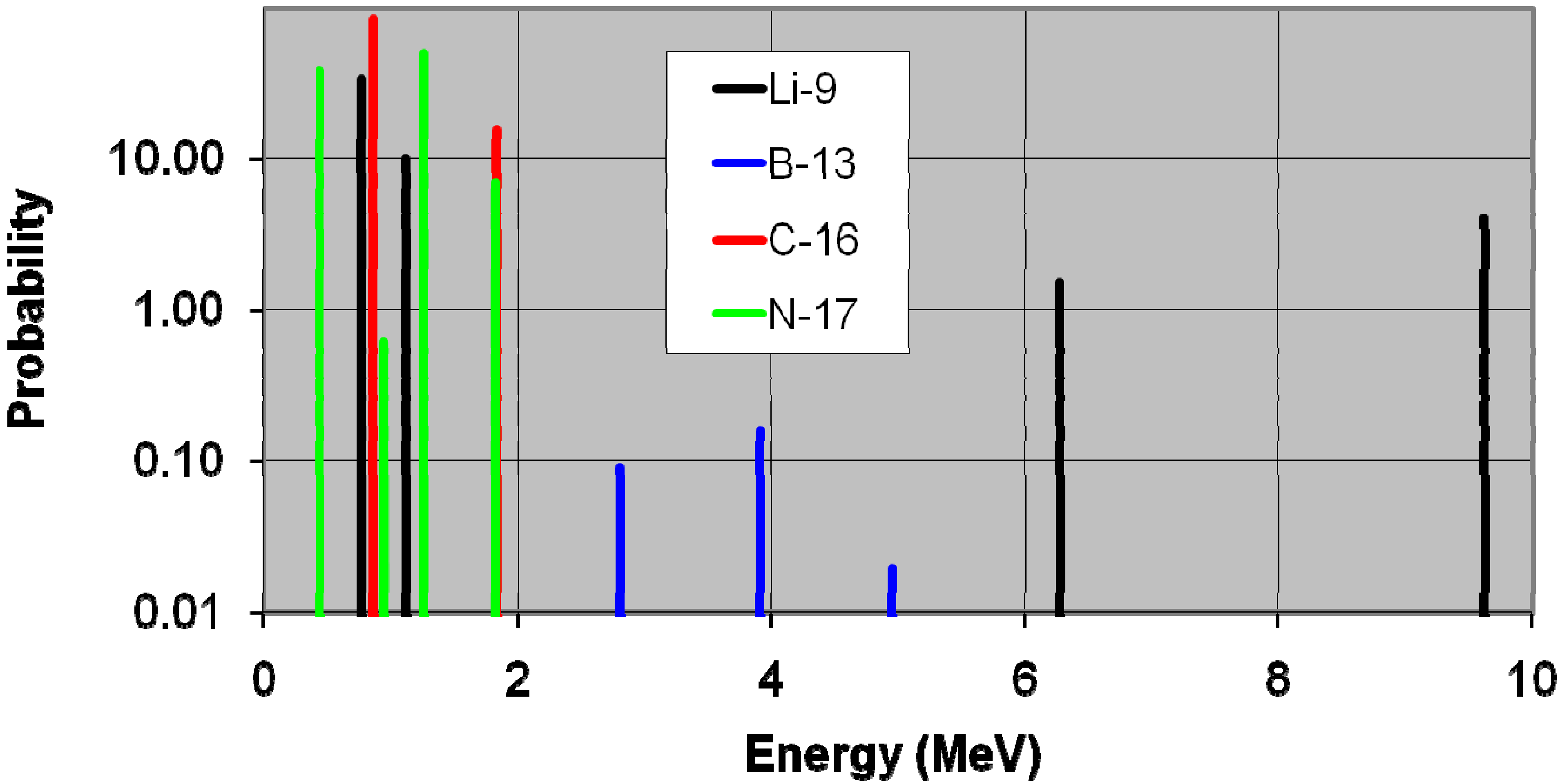

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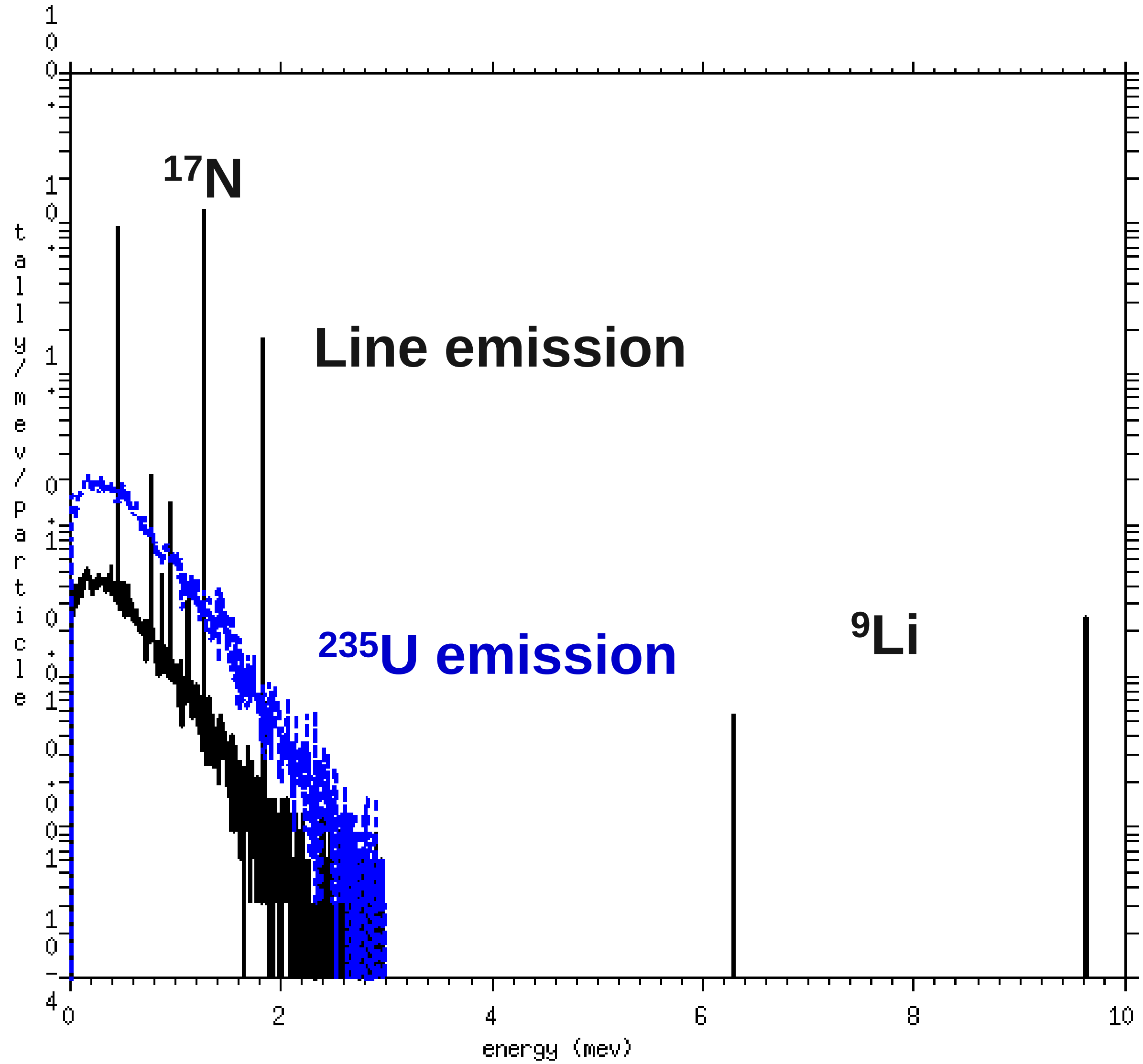
Delayed neutron spectra have also been calculated for lighter isotopes – neutron activation of low-Z nuclides

A small sphere of ^{9}Be,^{13}C, $^{17,18}O$, and , ^{235}U was irradiated by 14-MeV neutrons. Blue line shows the previous DN treatment (^{235}U spectrum used for all DN emission). Black line shows emission with line data.



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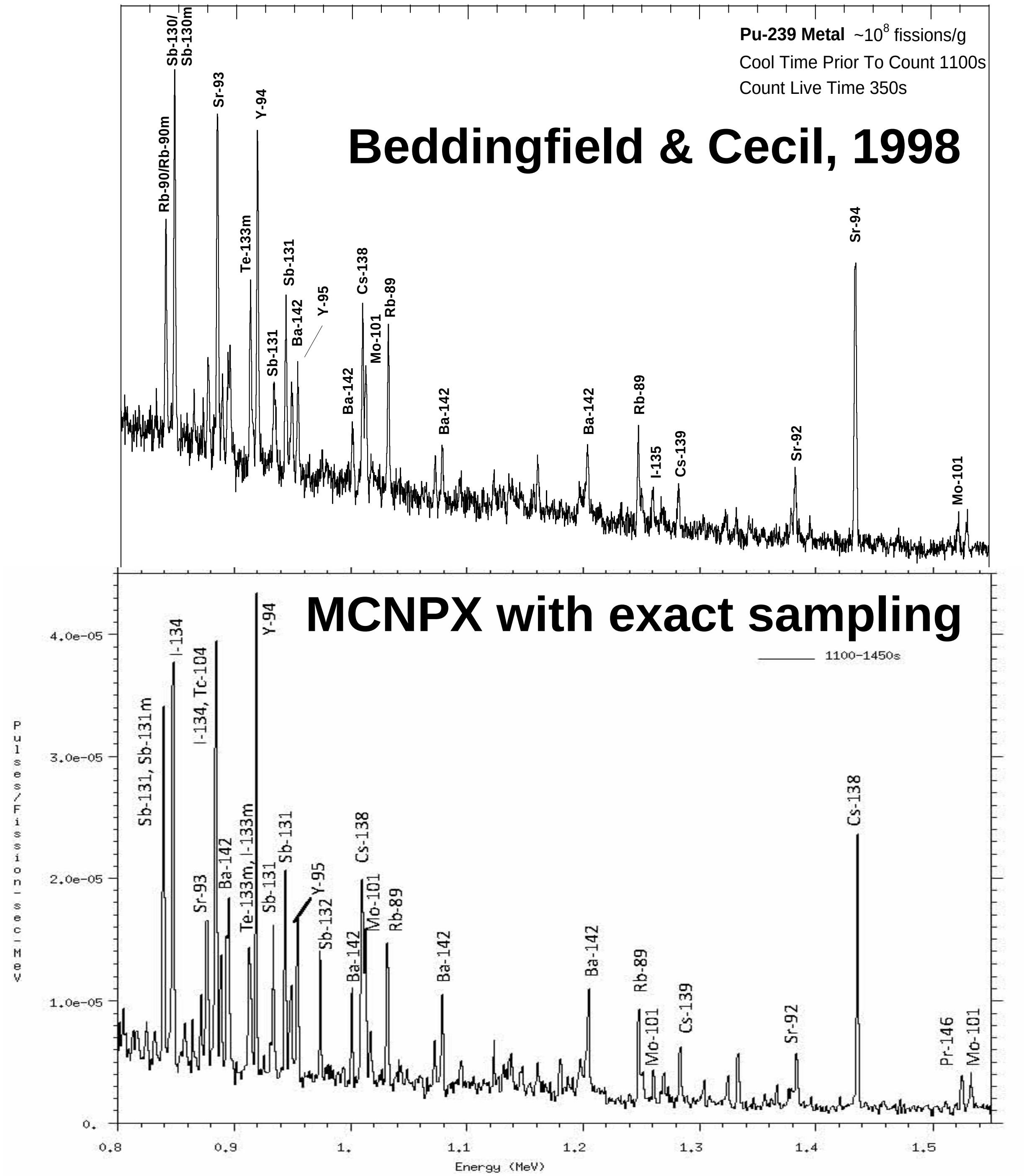
Validation Result

Delayed gamma spectroscopic results for neutron irradiation of a small disk of ^{239}Pu. MCNPX results are in good agreement with the measured data (obtained using a HPGe detector).



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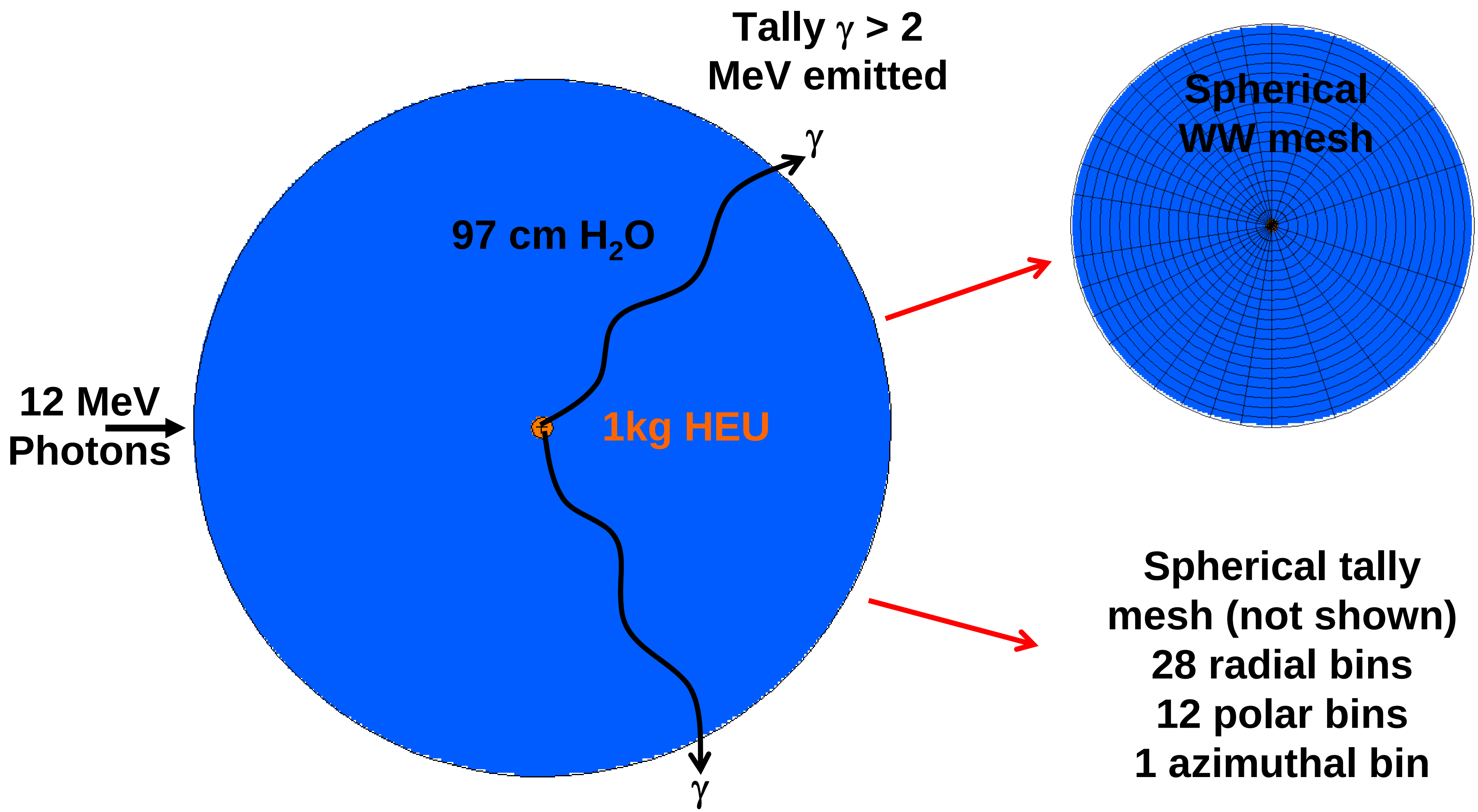
Spherical time-energy WW test problem involves photon interrogation of shielded HEU



Spherical tally mesh (not shown)
28 radial bins
12 polar bins
1 azimuthal bin

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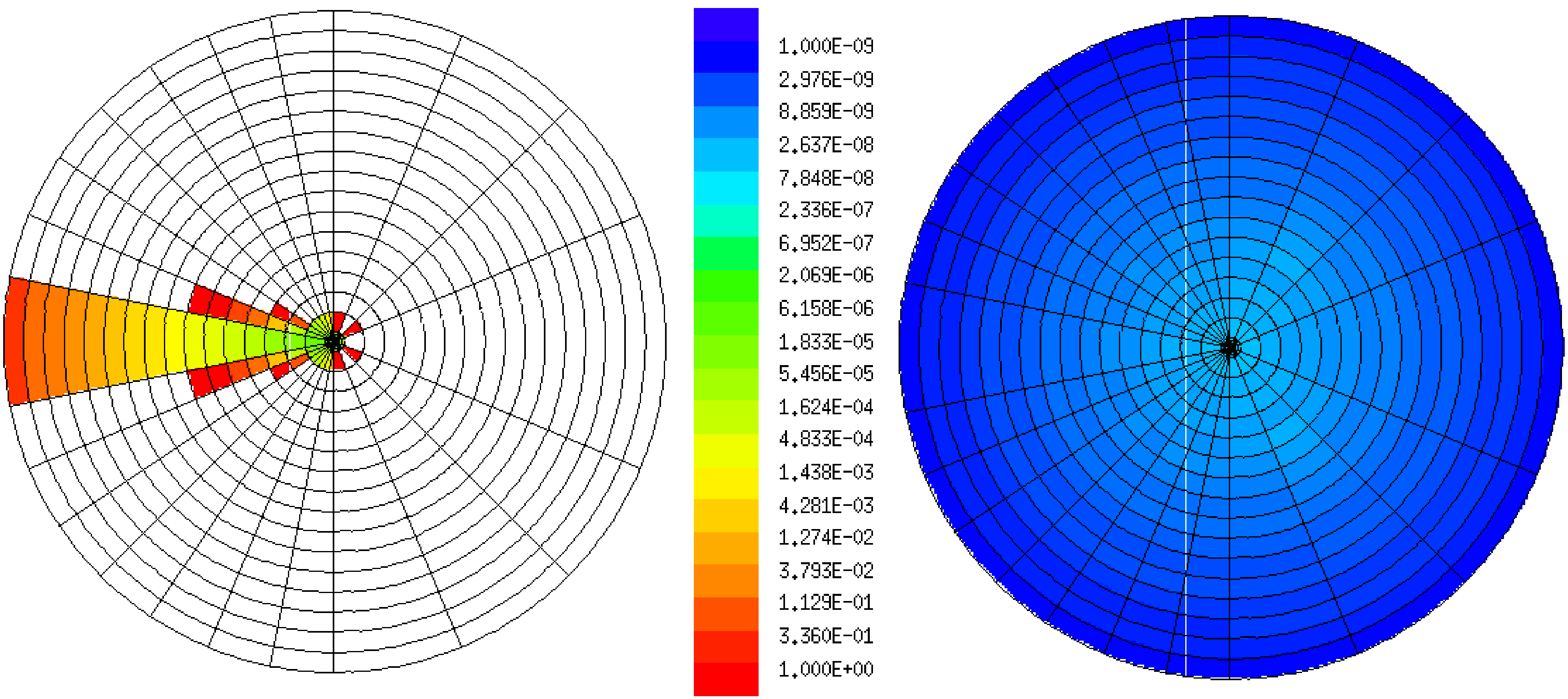
Spherical WW included two energy groups (low, high) and two time bins (prompt, delayed)

High energy prompt photon WW

High energy delayed photon WW



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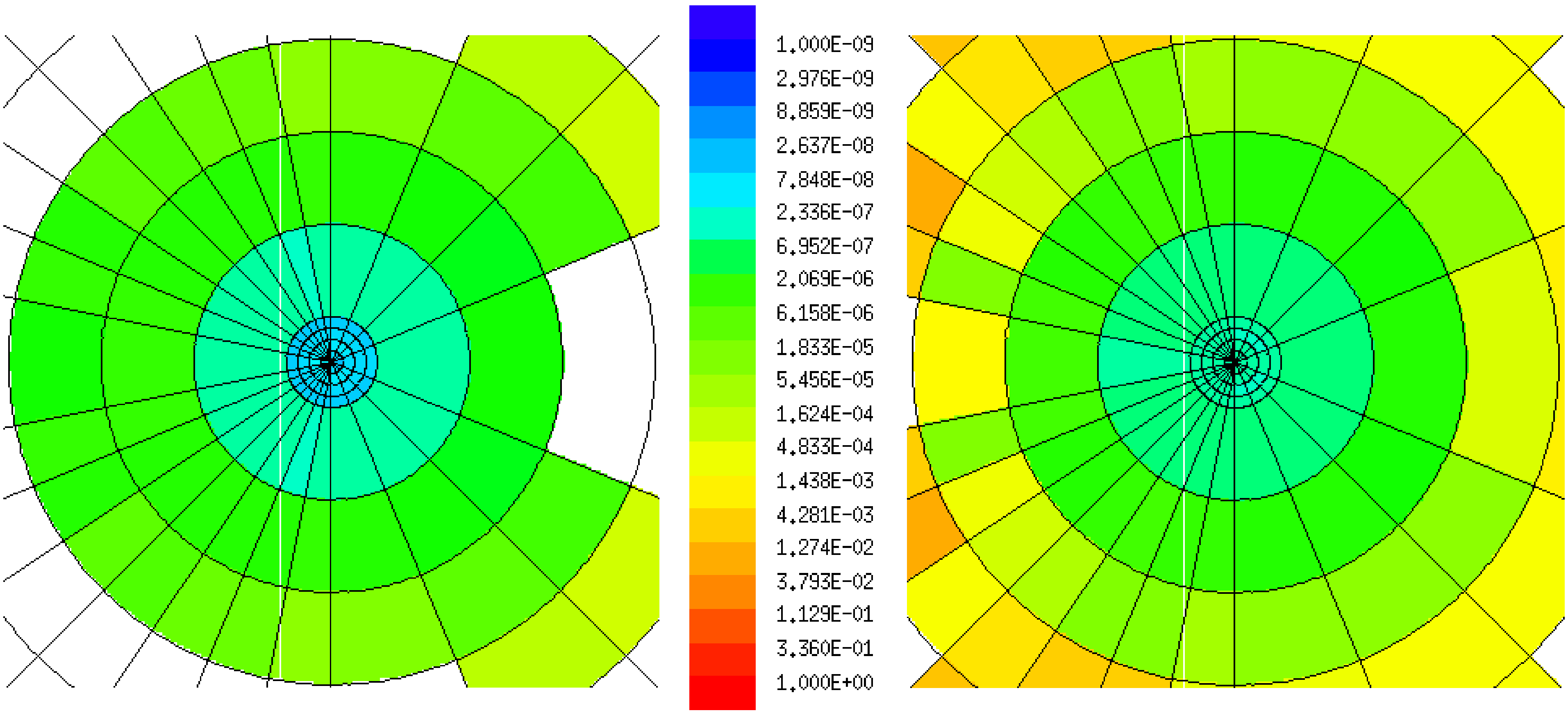
Spherical WW included two energy groups (low, high) and two time bins (prompt, delayed)

Low energy prompt neutron WW

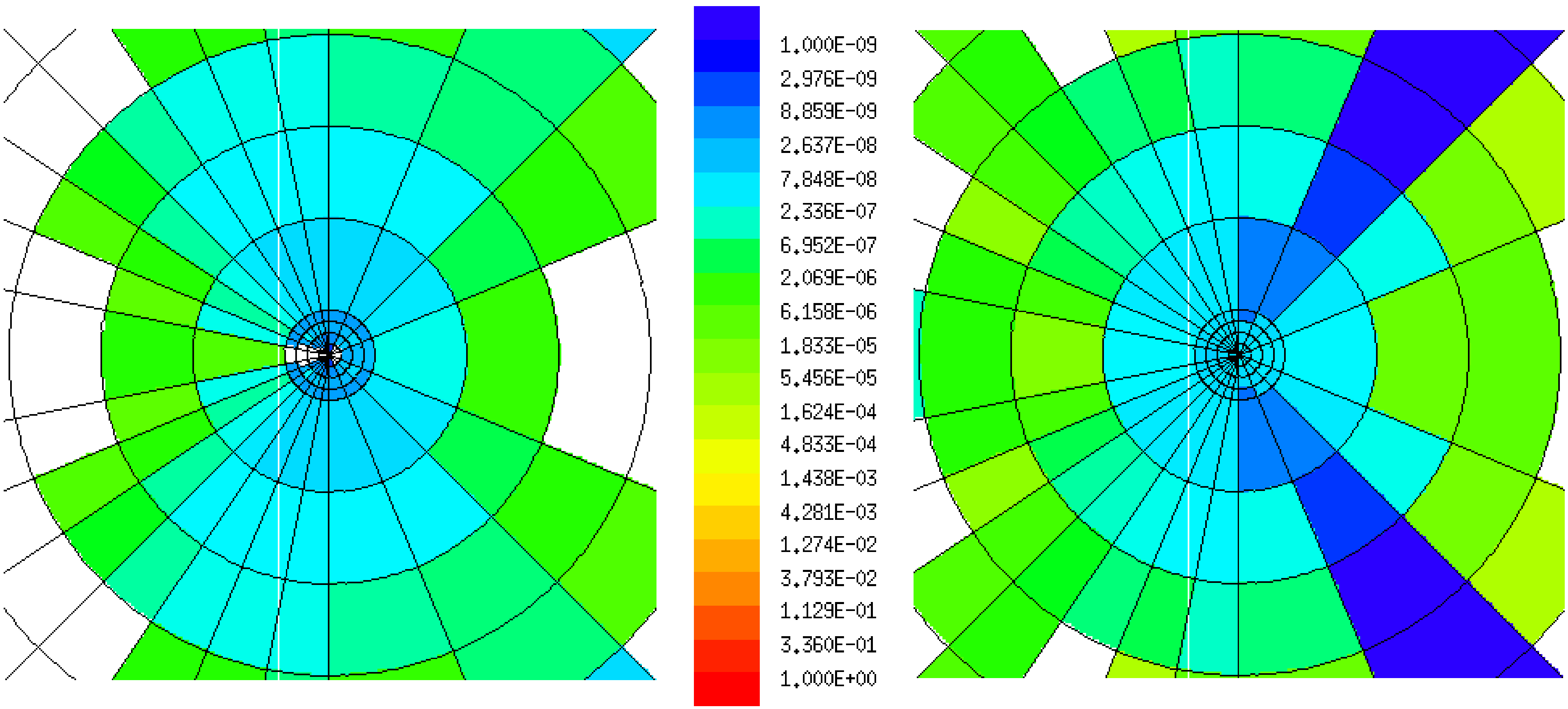
High energy prompt neutron WW



Spherical WW included two energy groups (low, high) and two time bins (prompt, delayed)

Low energy delayed neutron WW

High energy delayed neutron WW



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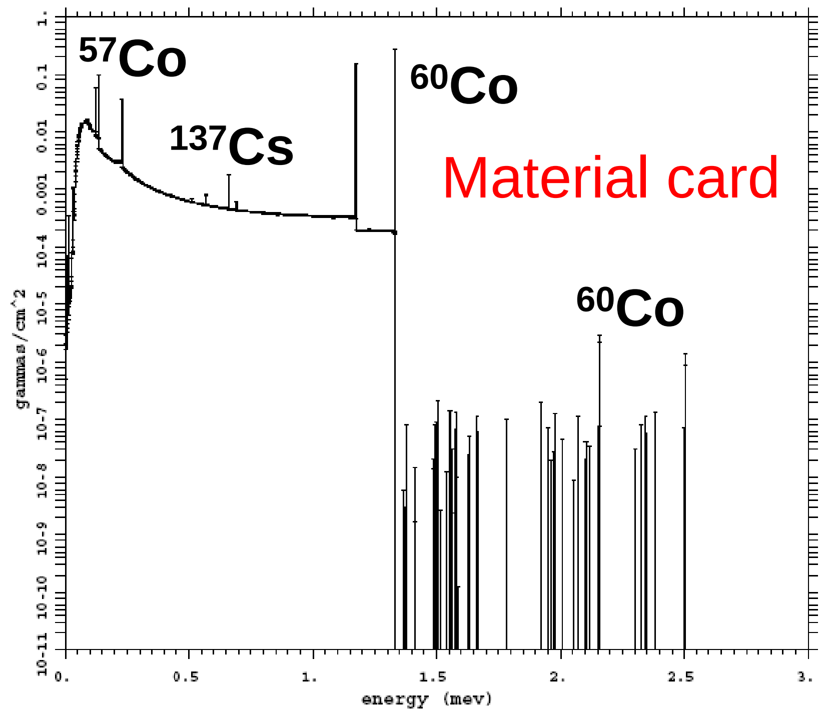
Radioactive sources can be mixed within standard materials – source strength is automatically calculated

```
Co-57, Co-60, & Cs-137 mixed in soil
1  1  -1.6   -1  imp:p=1
2  0          1  imp:p=0

1  so  100.0

mode p #
m1     1001 -.002  8016 -.527 11023 -.021
     13027 -.061 14028 -.345 19000 -.029
     26056 -.016 27057 -.00000001
     27060 -.000001 55137 -.000323
sdef par=sp pos=0 0 0 rad=d2
si2   0 100
sp2   -21 2
nps  100000000
phys:p 5j -102
f14:p 1
e14   0 999i 10
print
```



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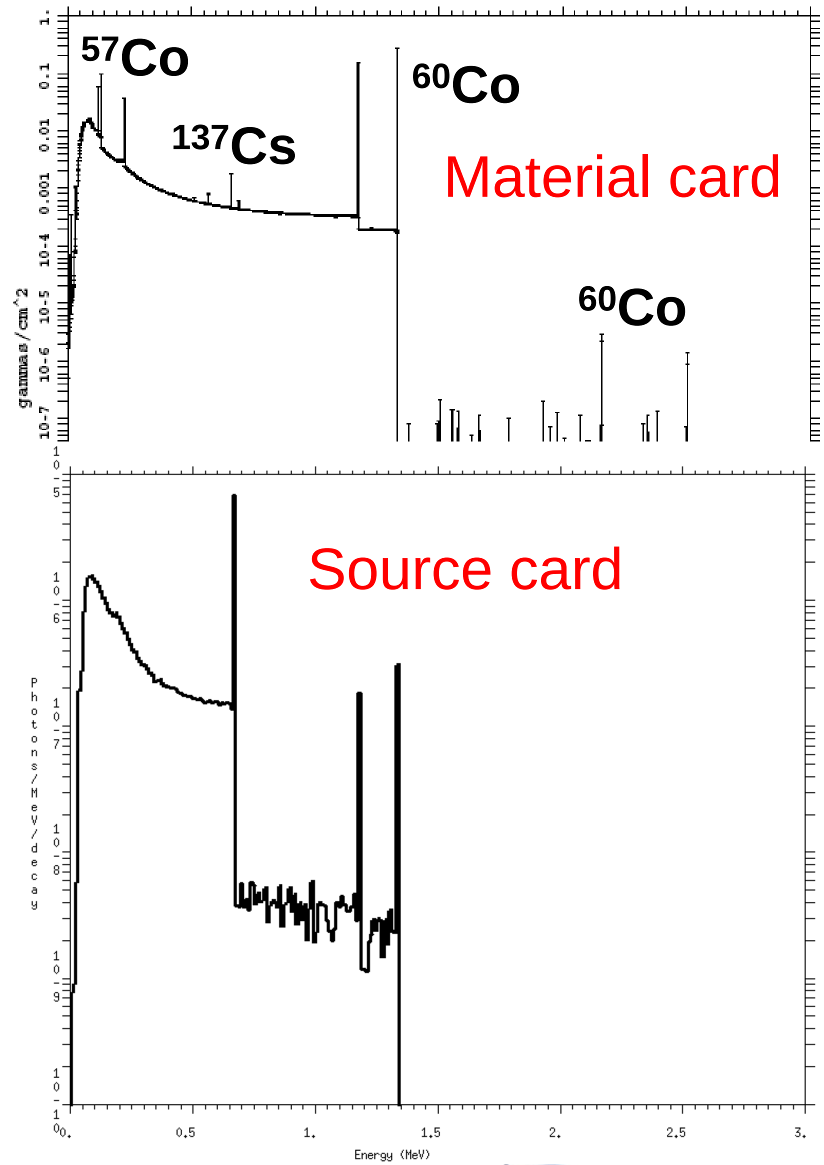
Radioactive sources can be combined with other standard sources – addresses issue of missing nuclear libraries

```
Co-57, Co-60, & Cs-137 using SDEF card
1  1  -1.6   -1  imp:p=1
2  0          1  imp:p=0

1  so  100.0

mode p #
m1     1001 -.002  8016 -.527 11023 -.021
     13027 -.061 14028 -.345 19000 -.029
     26056 -.016
sdef par=d1 erg=0 pos=0 0 0 rad=d2
si1 L      27057        27060        55137
sp1   0.00003086  0.00308632  0.99688281
si2   0 100
sp2   -21 2
nps  100000000
phys:p 5j -102
f14:p 1
e14   0 999i 10
print
```



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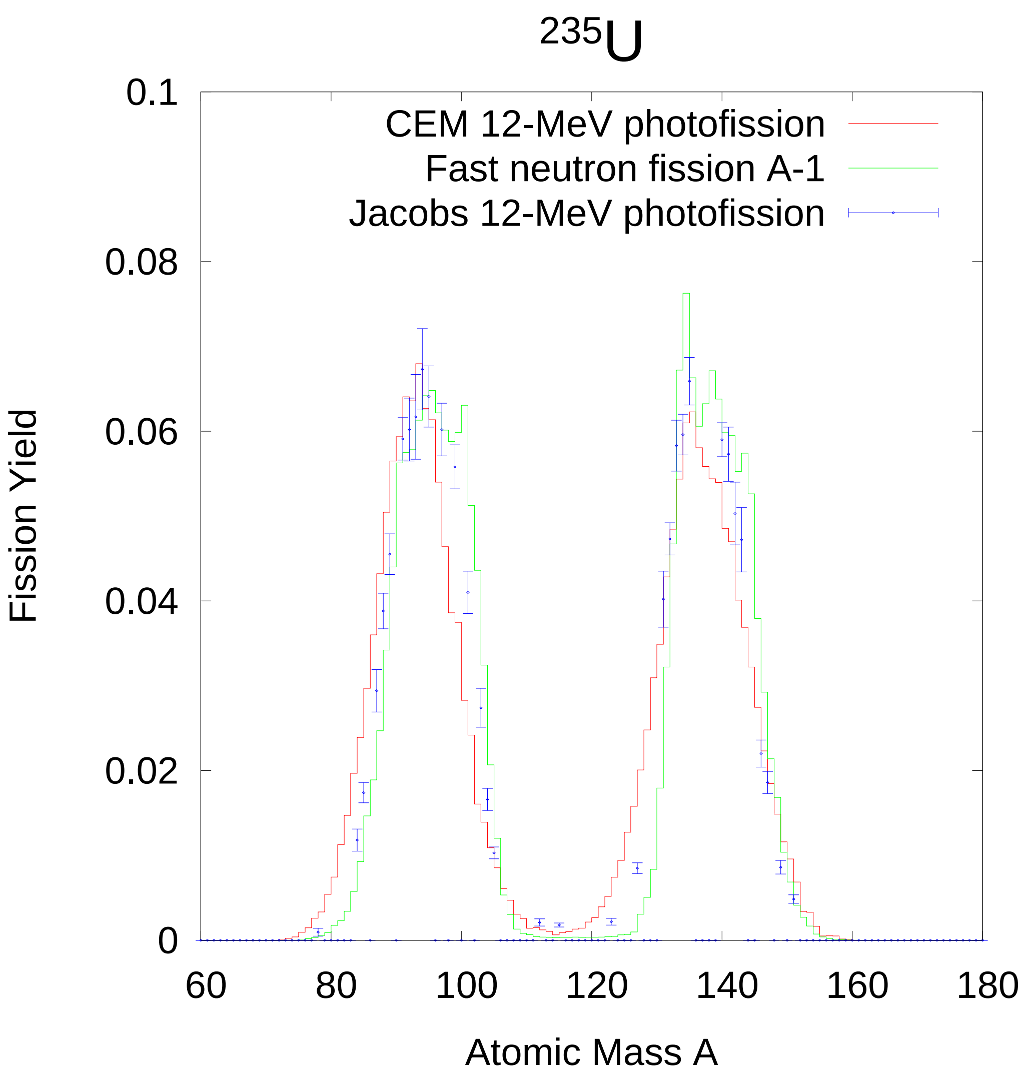
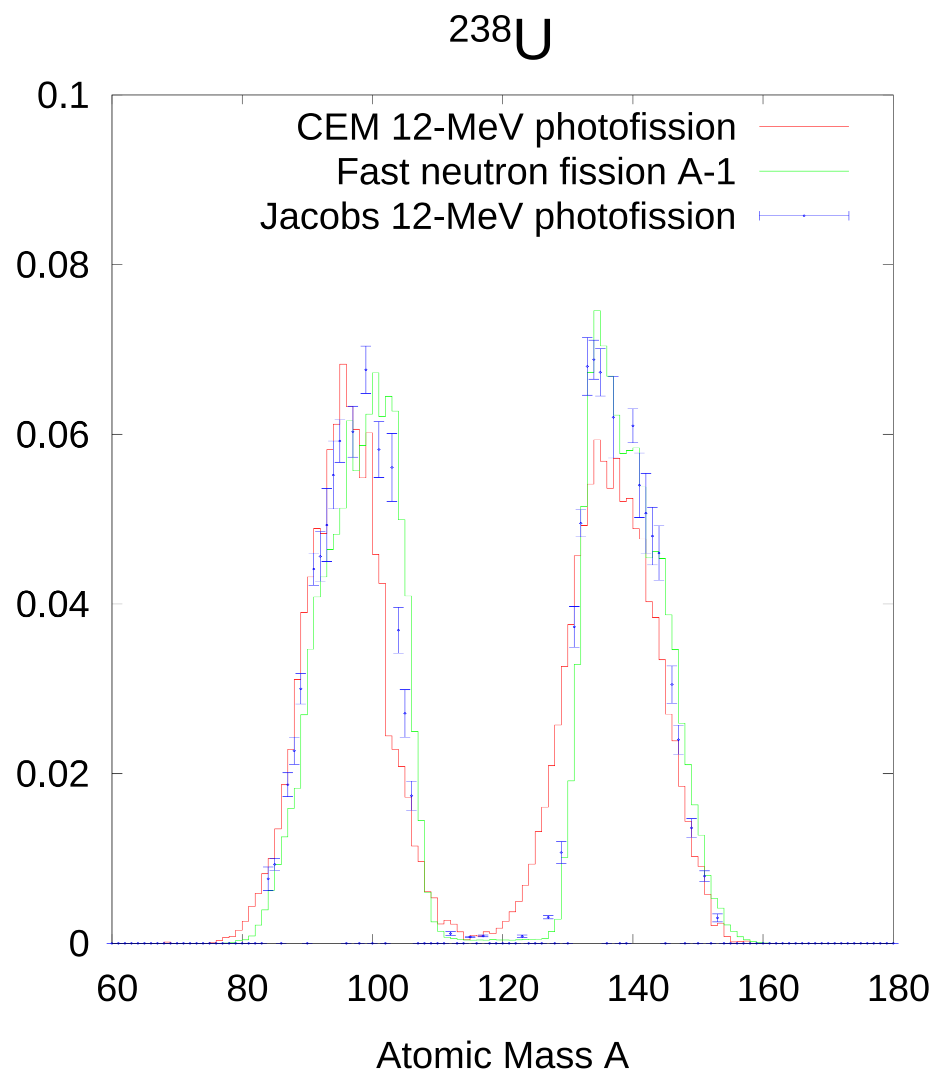
Photofission fission-product yields are no longer taken from neutron data – CEM used to produce new yields





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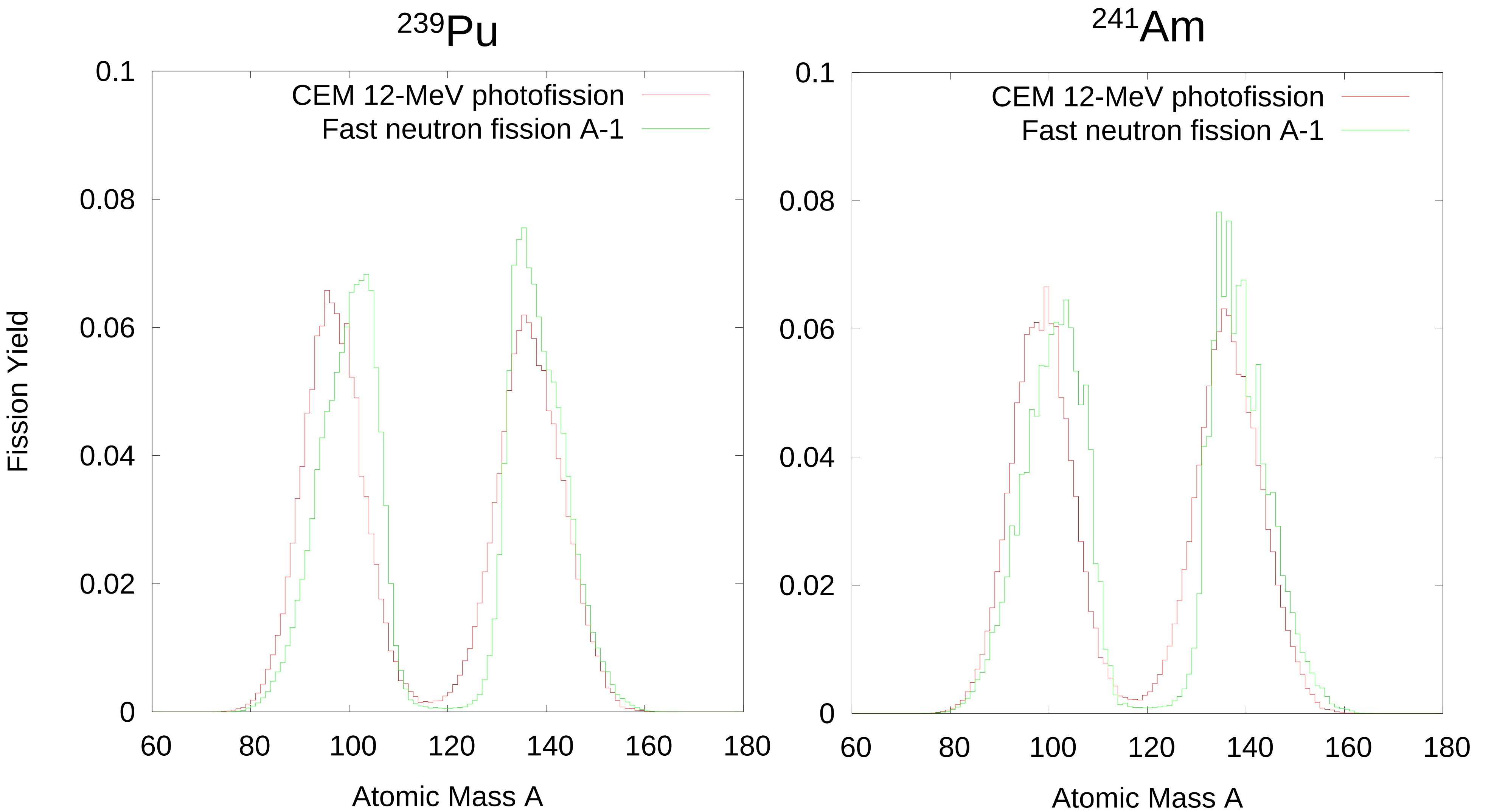

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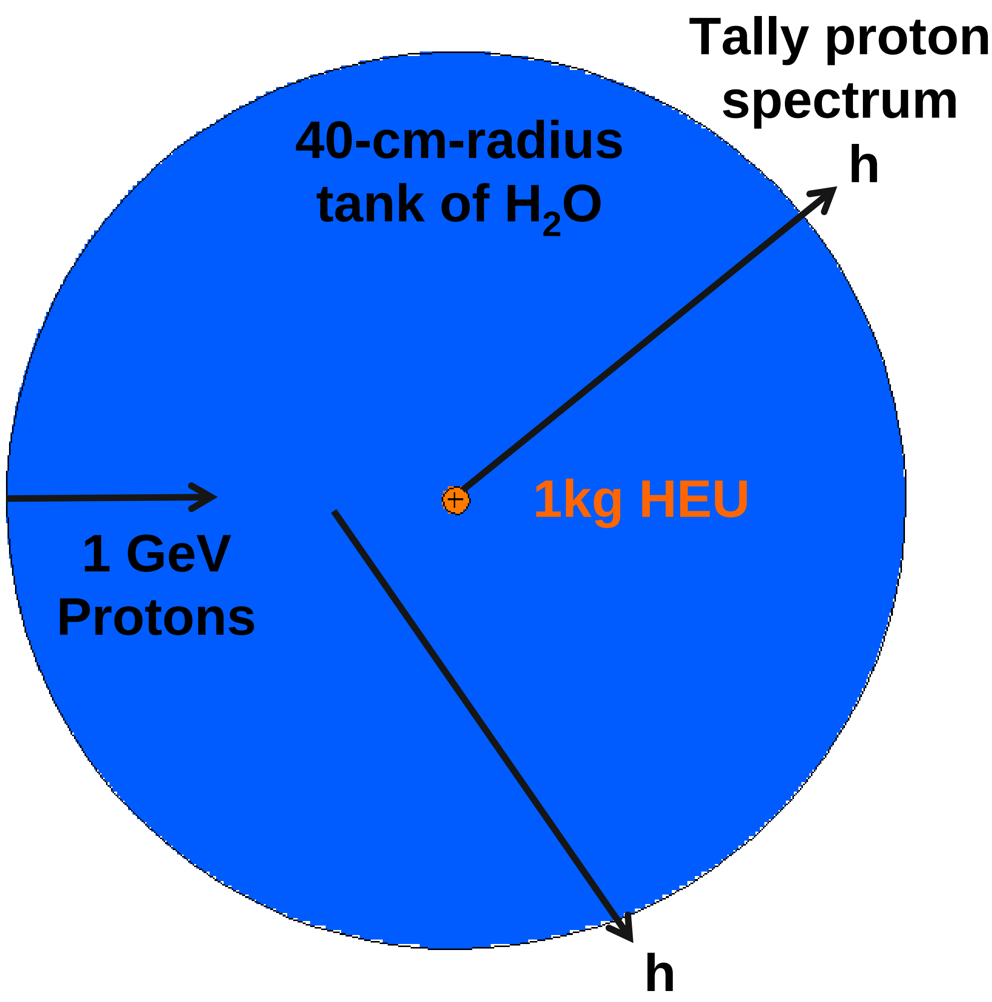
Proton tally tagging demonstrated on a shielded HEU test problem

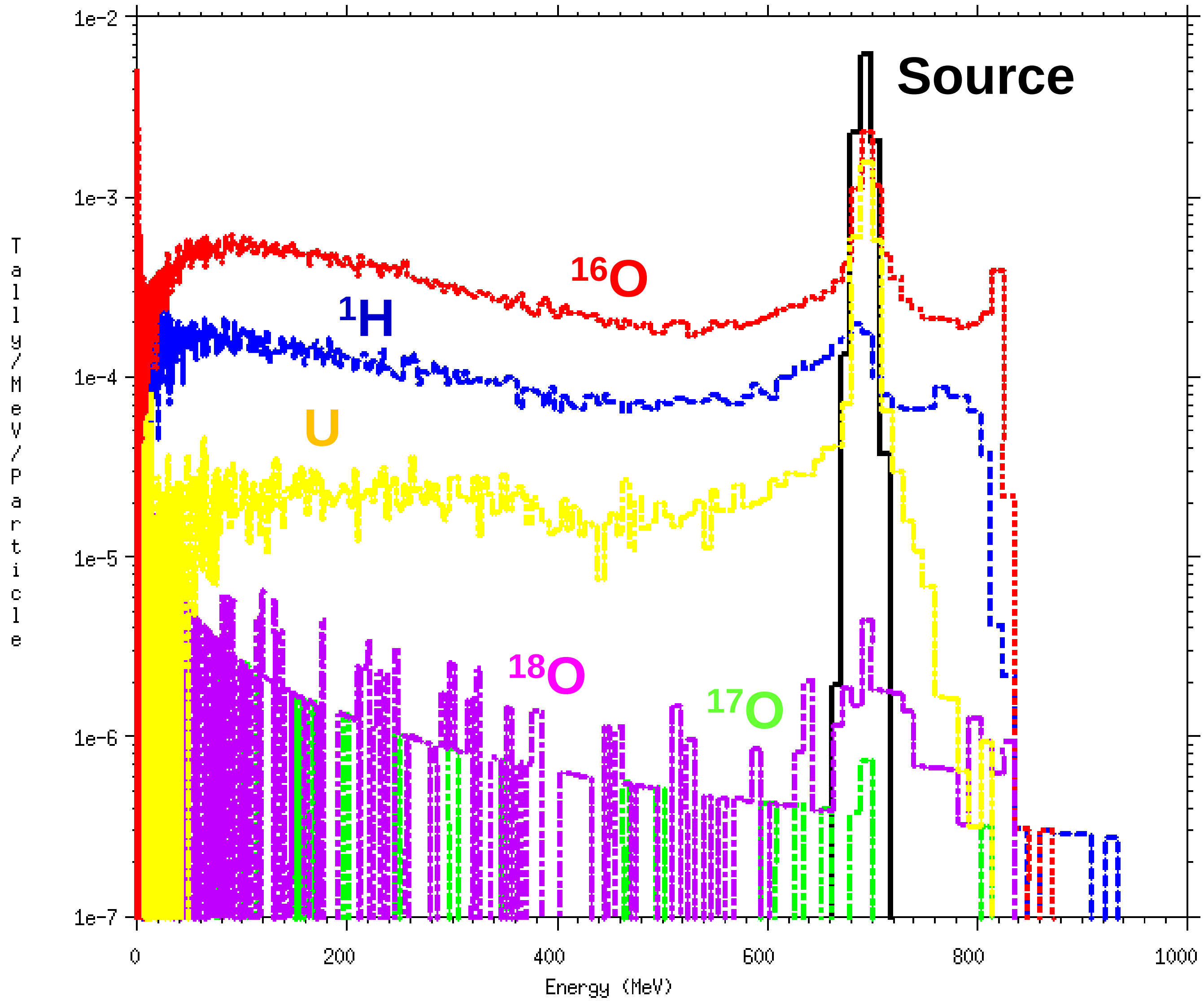
```
1-GeV protons into water + HEU
1  1 -19.0   -1      imp:n=1
2  2  -1.0    1 -2   imp:n=1
3  0             2   imp:n=0

1  so 3.0
2  so 40.0

m1      92235 100    92238 100
m2       1001 200    8016 99.762
         8017 0.038  8018 0.200
sdef    par=h erg=1000 pos=-39.99 0 0
        vec=1 0 0 dir=1
mode    h n p / z
phys:n 1001
cut:h   j .001
f1:h    2
e1      1e-3 999log 1000
ft1     tag 3
fu1     -1.0 1001.0
        8016.0  8017.0  8018.0
        92235.0  92238.0 1e10
print
nps     1000000
```



Proton tagging for a shielded HEU test problem – components of the escape spectrum



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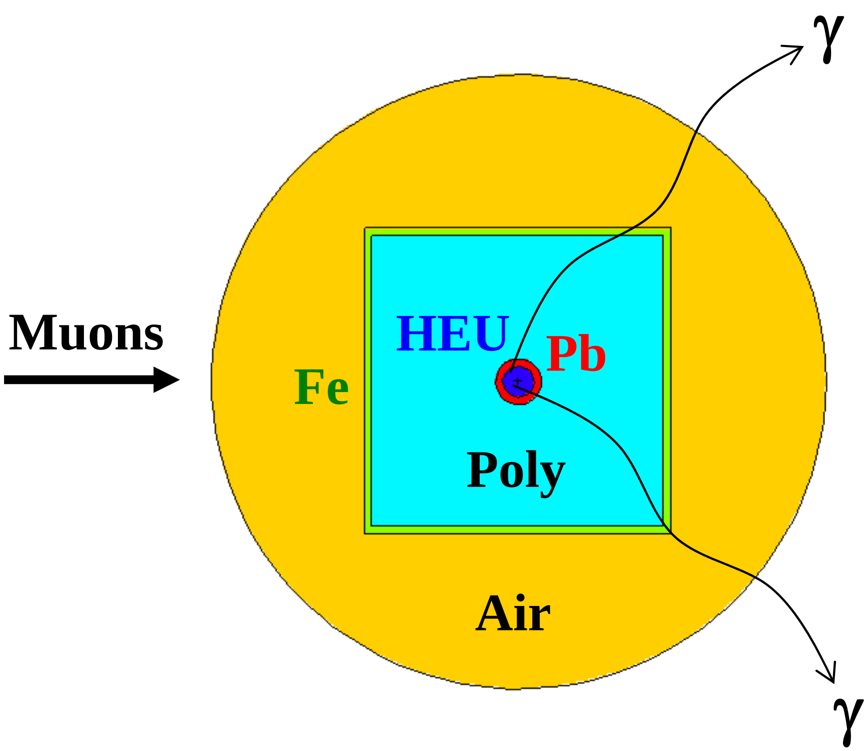
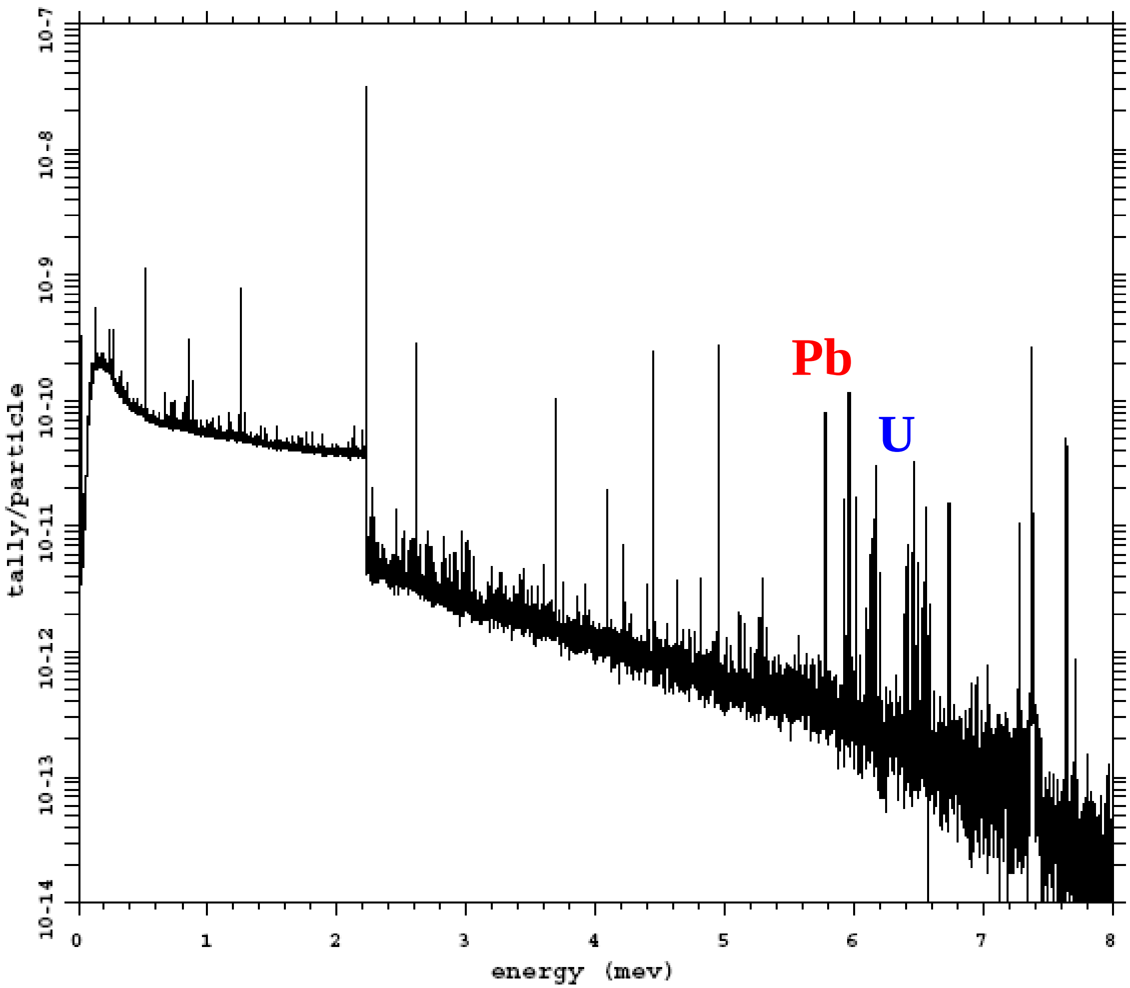
X-ray spectrum from 350-MeV muons interrogating shielded HEU





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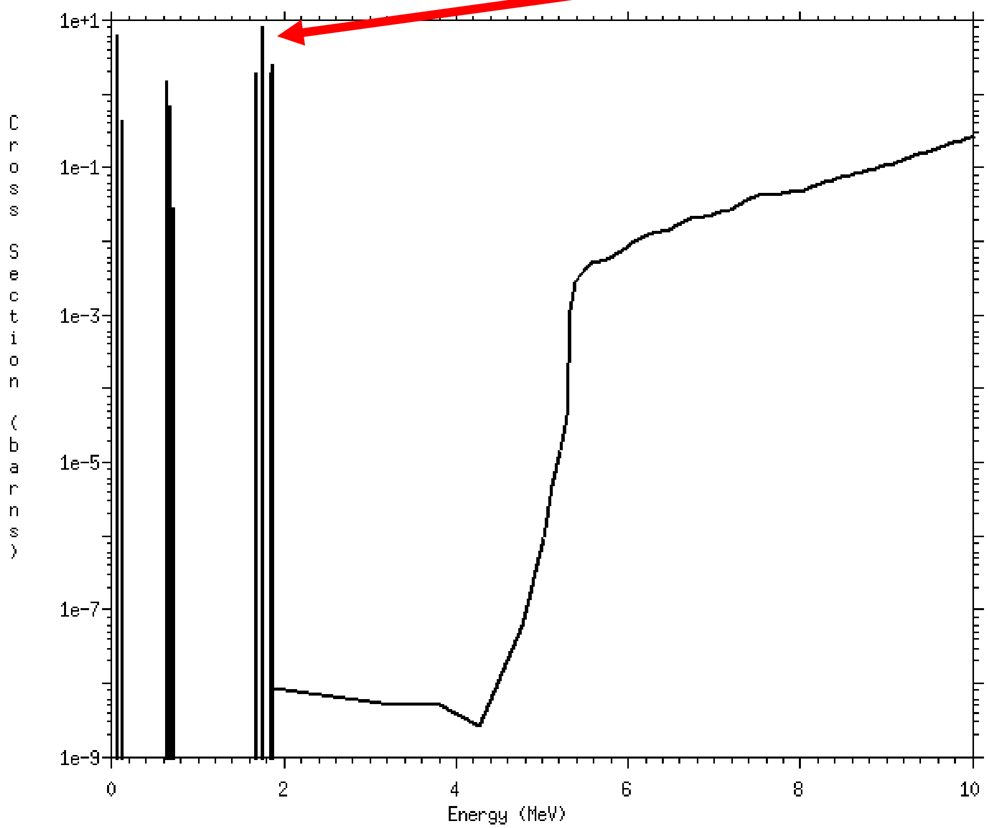
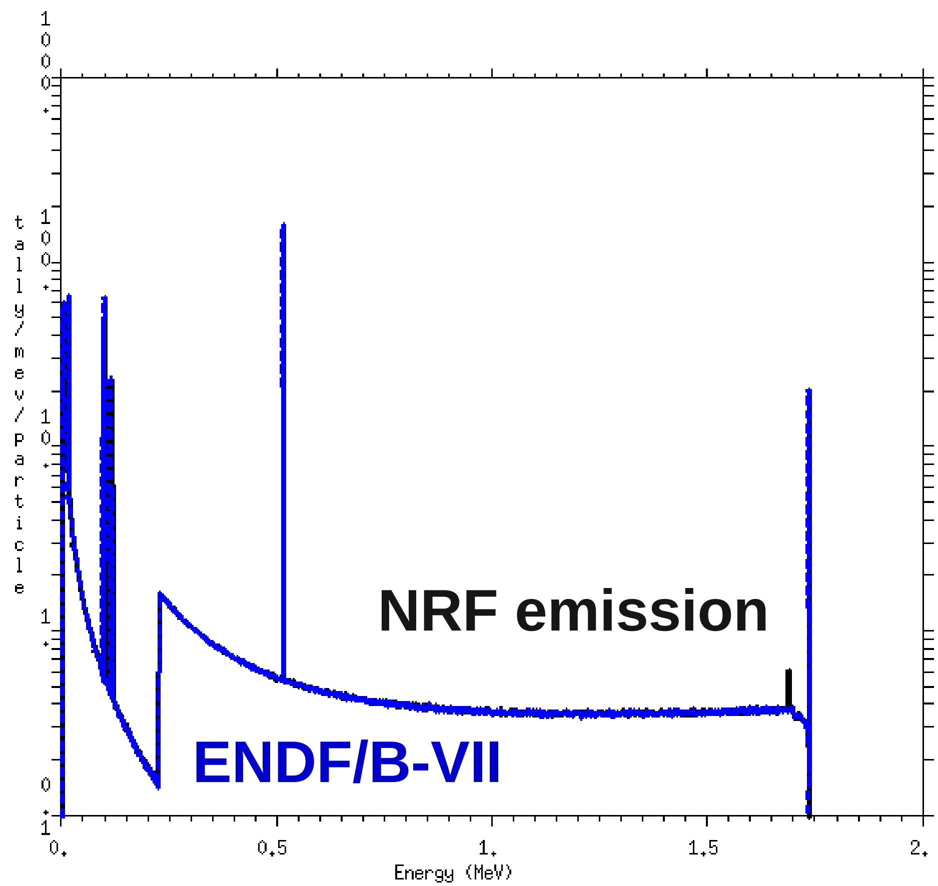
NRF data collected from various sources – resonances replace existing absorption cross section (^{235}U)

ACE library with NRF resonances

Gamma spectrum emitted with 1.7330 MeV γ incident

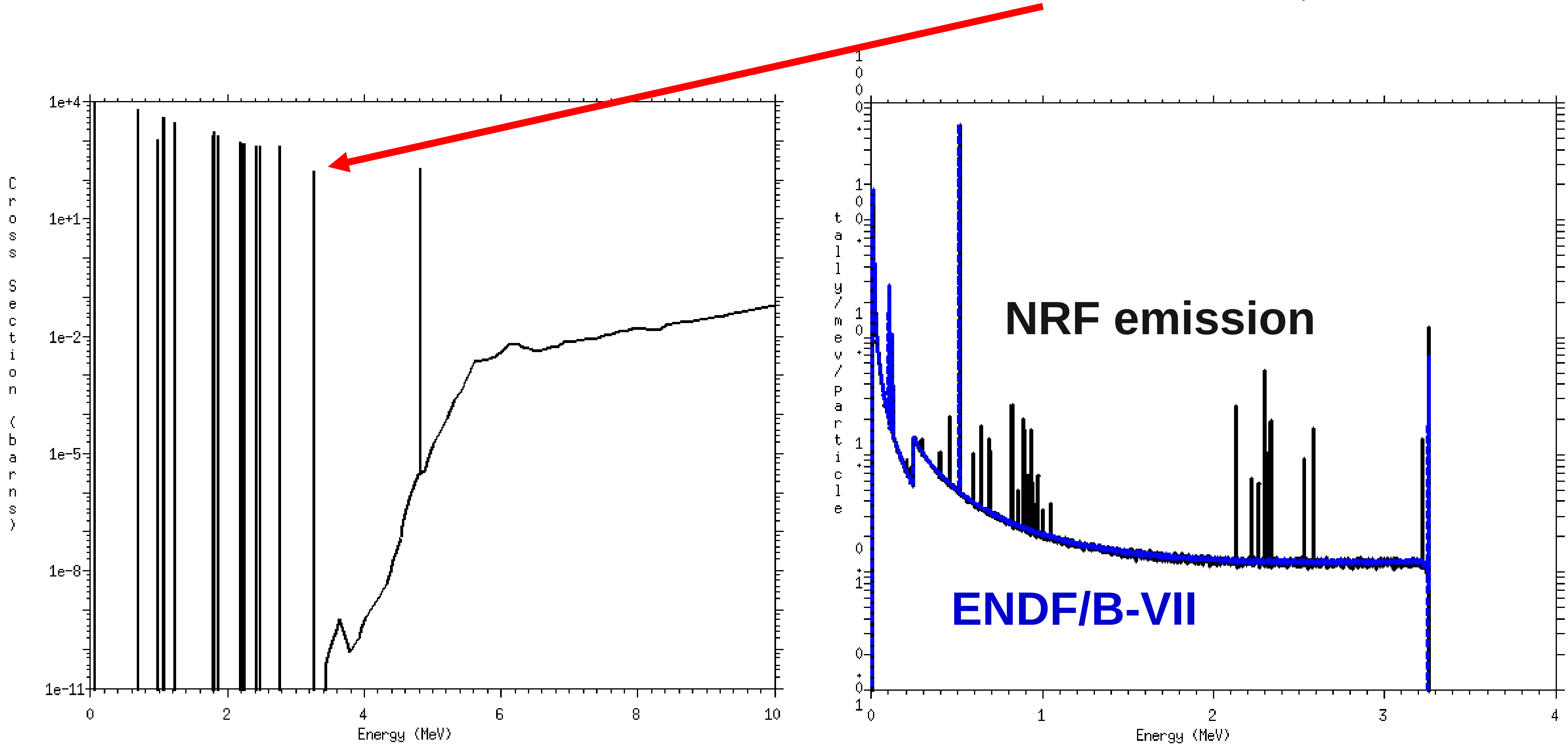




NRF data collected from various sources – resonances replace existing absorption cross section (^{238}U)

ACE library with NRF resonances

Gamma spectrum emitted with 3.2534 MeV γ incident



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