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Title: MCNP5 + Data + MCNPX Workshop

Author(s): Forrest B. Brown, Albert C. Kahler, Gregg W. McKinney, Russell D. Mosteller, Morgan C. White

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ANS Mathematics & Computation Topical Meeting
Monterey, CA, 15-19 April 2007

LA-UR-07-2053

MCNP5 + Data + MCNPX Workshop

Forrest Brown, Skip Kahler, Gregg McKinney,
Russ Mosteller, Morgan White

Los Alamos National Laboratory

Abstract

MCNP5 + Data + MCNPX Workshop

F.B. Brown, A.C. Kahler, G.W. McKinney, R.D. Mosteller, M.C. White
Los Alamos National Laboratory

This workshop provides an overview of recent advances in Monte Carlo particle transport codes and data at Los Alamos National Laboratory.

The MCNP5 and MCNPX Monte Carlo codes are used worldwide for particle transport calculations for reactors, radiation shielding, accelerators, medical physics, dosimetry, homeland security, experiment analysis, and many other applications. Updates are provided on the status and recent progress for each code.

Transport codes are only as good as the cross-section data they use. One of the most significant computational events of this year is the introduction of the ENDF/B-VII nuclear datasets. The extensive work in evaluating, preparing, and testing the data over the past few years will be described, along with some remaining challenges. Plans for making the ENDF/B-VII data available to MCNP5 and MCNPX users will also be presented.

MCNP5 + Data + MCNPX Workshop

F.B. Brown, A.C. Kahler, G.W. McKinney, R.D. Mosteller, M.C. White

- **MCNP5 Advances** **(Brown, .5 hr)**
  - Status & current work
  - Performance: multi-core threading, clusters

- **ENDF/B-VII Data** **(Kahler, Mosteller, White, 1.5 hr)**
  - Why ENDF/B-VII; What was wrong with ENDF/B-VI?
  - Processing ENDF/B-VII neutron files into an MCNP Library
  - Data Testing with ICSBEP Benchmarks
  - What's improved, what deficiencies remain?
  - Plans for release of MCNP ENDF/B-VII libraries

- **MCNPX Advances** **(McKinney, .5 hr)**
  - Overview of MCNPX 2006-2007 Features
  - Decay Particle Production from Fission & Activation
  - Coupled Space, Energy, Time Spherical Weight Windows
  - Background Radioactive Sources

LA-UR-07-2053

MCNP5 Advances

Forrest B. Brown

Monte Carlo Codes (X-3-MCC)
Los Alamos National Laboratory
`fbrown@lanl.gov`

MCNP5 Advances

- **MCNP5 Releases**
  - Status
  - New features
- **MCNP5/6 - Ongoing work**
  - MCNP6 / MCNPX merger
  - Major revisions to classes
  - Acceleration & convergence for criticality problems
- **MCNP5 Performance**
  - Compilers & Threading

MCNP5 Releases

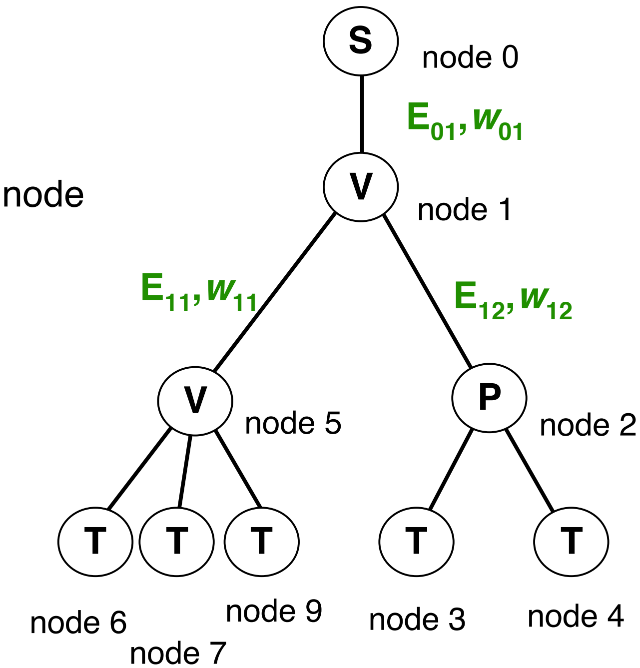
- **Current, RSICC: MCNP5 / 1.40 (Spring 2006)**
  - Lethargy plots for energy dependent tallies
  - Logarithmic interpolation for input data
  - Fission neutron multiplicity
  - Stochastic geometry
  - Source entropy with plots
  - Mesh tally plotter
  - New electron energy-loss straggling logic
  - Source particle type specification
  - Positron sources
- **Nearing completion: MCNP5 / 1.50 (Spring 2007)**
  - **Variance reduction for pulse height tallies (F8)**
  - **MAKXSF - Doppler broadening & temperature interpolation**
  - Long filenames
  - Numerous minor bug fixes
- **Planned: new data (Summer 2007 ?)**
  - ENDF/B-VII.0 data libraries in ACE format

- **Pulse height tallies (F8) depend on collections of particles (e.g., the entire particle history)**
  - Two 1 MeV photons deposited in one cell registered as one 2 MeV count, not two 1 MeV counts
  - Assumes both photons have weight one
  - Not the case when using variance reduction
- **Create "trees" to keep track of relationship between individual particles**
  - Weight assigned to branches of the tree
  - Energy deposited and weight stored for each branch

MCNP5 / 1.50 - Pulse Height Tally Variance Reduction

Monte Carlo Codes
X-3-MCC, LANL

S Source node
V Variance reduction node
P Physical node
T Terminal node



Pulse height tallies require knowledge of the entire particle history

E_{ij} is the energy deposited on $branch_{ij}$
w_{ij} is the weight multiplier for $branch_{ij}$

- **Variance reduction permitted**

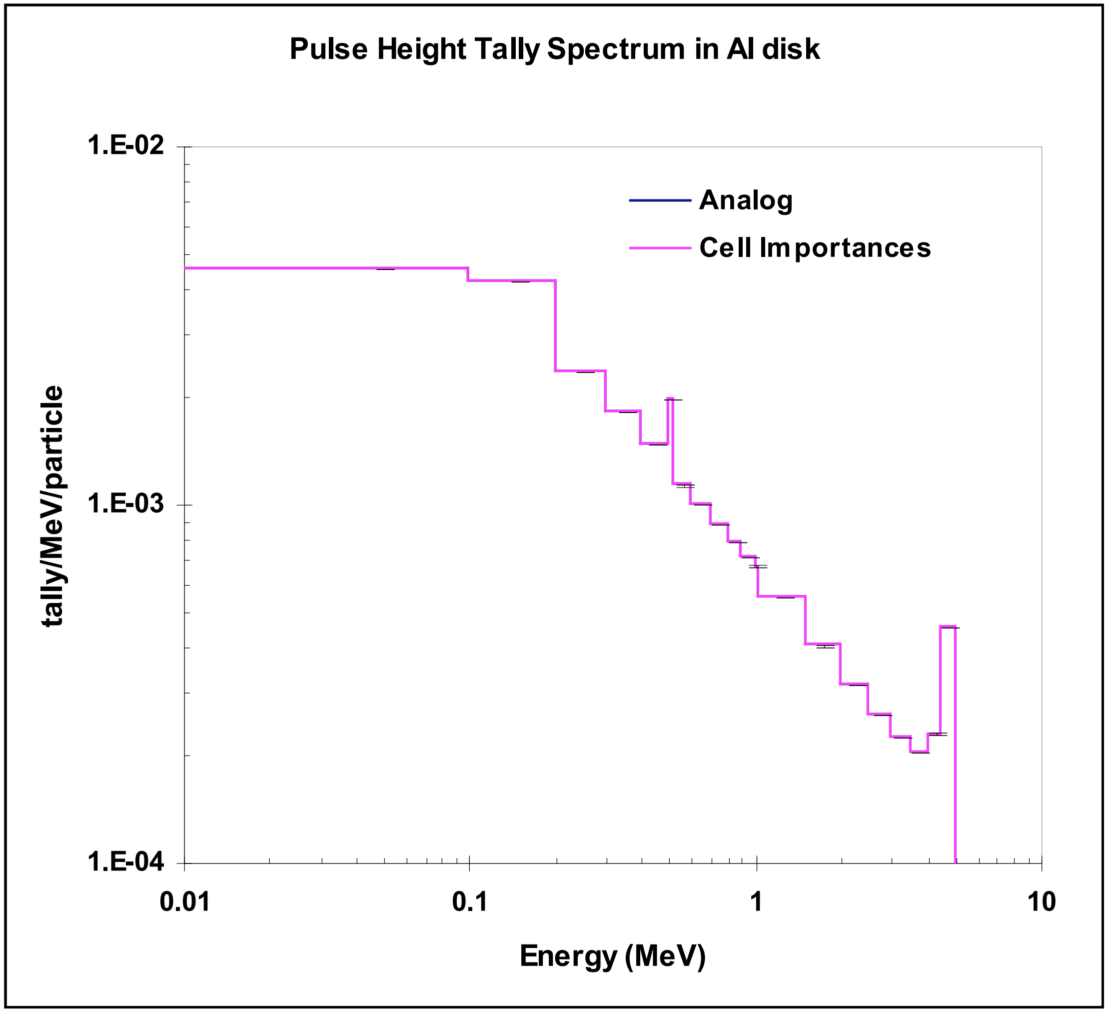
Geometry splitting	Energy splitting	Time splitting
Weight Window	Exponential Transform	Forced Collision
DXTRAN	Weight Cutoff	Implicit Capture

- **Variance reduction NOT permitted**
  - Neutrons
  - Electron specific variance reduction that controls types and how many specific types of electrons are produced:

Bremsstrahlung	photon-induced secondary electrons
electron-induced x–rays	knock-on electrons

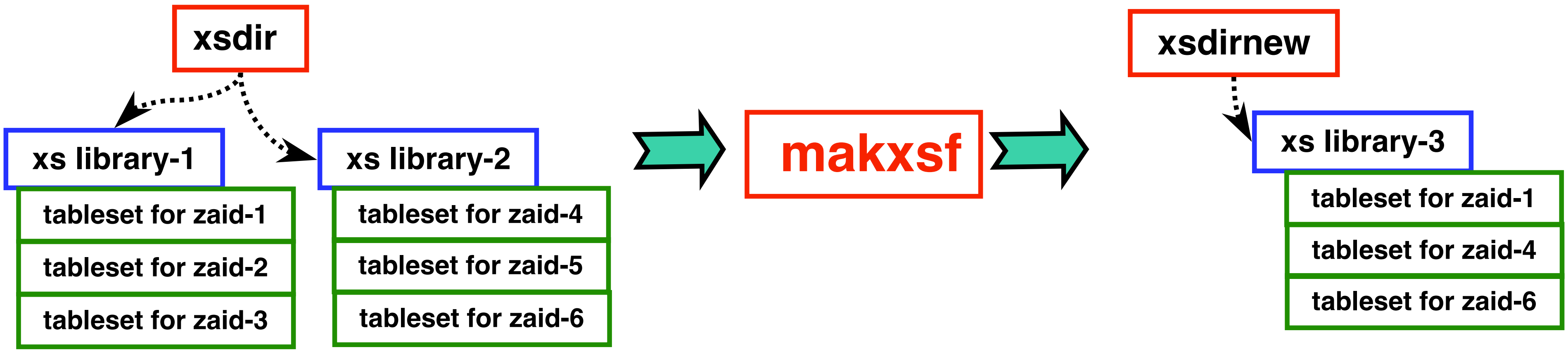
MCNP5 / 1.50 - Pulse Height Tally Variance Reduction

- 100 cm x 100 cm cylinder
- 10 cm thick disks
- Two Aluminum disks followed by one Oxygen disk
- 5 MeV isotropic photon source at the base
- Tally in final Al slab (90-100 cm)



MCNP5 / 1.50 - makxsf

Monte Carlo Codes X-3-MCC, LANL



- **Traditional MAKXSF functions**
  - Convert cross-section libraries to/from ASCII & binary
  - Copy entire libraries to new files
  - Copy selected nuclide tablesets to new libraries
  - Create new **xsdir** file for the new libraries
- **Create nuclide table-sets at new temperatures** [new]
  - **Doppler broaden resolved resonance data to higher T**
  - **Interpolate unresolved resonance probability tables to new T**
  - **Interpolate S(α,β) thermal data to new T**

MCNP5 / 1.50 - makxsf

- **Taken from "doppler" code by MacFarlane, taken from NJOY**
    1. R.E. MacFarlane & P. Talou, "DOPPLER: A Utility Code for Preparing Customized Temperature-Dependent Data Libraries for the MCNP Monte Carlo Transport Code", unpublished (Oct 3, 2003)
    2. R.E. MacFarlane & D.W. Muir, "The NJOY Nuclear Data Processing System, Version 91", LA-12740-M (1994).

- **Doppler**
    - **Doppler broaden the resolved resonance data** to new (higher) temperature
    - Temperatures can be specified in degrees-K or in MeV
    - Only need base cross-section, at lower temperature

- **Interpolation**
    - For **S(α,β) thermal data** or **unresolved resonance probability table** data
    - Must have existing datasets at BOTH lower & higher temperature

- **Mosteller, MacFarlane, Little, White, "Analysis of Hot and Cold Kritz Benchmarks With MCNP5 and Temperature-specific Nuclear Data Libraries", LA-UR-03-7071 (2003).**
  - Separate nuclear data sets were generated at 245 C using DOPPLER and NJOY
  - Basic data were taken from ENDF/B-VI Release 6 (ENDF66)
  - **MCNP5** calculations were performed for the hot 2-D benchmarks, and the results were compared
  - Each calculation employed 550 generations with 10,000 neutron histories per generation
  - Results from first 50 generations were discarded, giving 5,000,000 active histories for each case

Case	Library	keff	Δk (vs NJOY)
Kritz:2-1	NJOY	0.9914 ± 0.0003	—
	DOPPLER	0.9911 ± 0.0003	-0.0003 ± 0.0004
	new MAKXSF	0.9913 ± 0.0003	-0.0001 ± 0.0004
Kritz:2-13	NJOY	0.9944 ± 0.0003	—
	DOPPLER	0.9942 ± 0.0003	-0.0002 ± 0.0004
	new MAKXSF	0.9940 ± 0.0003	-0.0004 ± 0.0004
Kritz:2-19	NJOY	1.0005 ± 0.0003	—
	DOPPLER	1.0009 ± 0.0003	0.0004 ± 0.0004
	new MAKXSF	1.0004 ± 0.0003	-0.0001 ± 0.0004

MCNP5/6 Ongoing Work

- **MCNP6 - MCNPX Merger**
  - Happening now
  - Preserve features of both codes
  - Internal versions available this year
  - Will undergo extensive cleanup, testing, V&V
- **MCNP Classes**
  - Major upgrades to lectures
  - CD format, with extra references
- **Acceleration & convergence testing for criticality problems**
  - Improved tests using Keff & Shannon entropy of source distribution
  - Wielandt acceleration (paper this conference)
  - Fission matrix (& variants)

MCNP5 - Compilers & Threads

Monte Carlo Codes
X-3-MCC, LANL

- **MCNP5 performance - both serial & parallel - depends strongly on the Fortran-90 compiler & options used**
  - Runtime factors of 2-4x with <u>different compilers</u> on same hardware
  - Runtime factors of 2-4x with <u>different options</u> on same hardware & compiler
- **Parallel performance**
  - MCNP5 has always supported parallel calculations with **message-passing** (MPI, PVM) & **threading** (OpenMP)
  - Prior to mid-2006, Fortran compilers for Windows/Linux/Mac did a terrible job at threading. We recommended using only MPI.
  - Recently, using OpenMP threading with Intel compilers on Windows/Linux/Mac shows excellent speedups -- nearly 2x on dual-cores.
- **Examples & demo for MacBook Pro (Core2 Duo)**
  - KCODE: BAWXI2 benchmark, kcode 5000 1 10 50
  - Fixed source: inp12, oil-well log, mode n, nps 105000

MCNP5 - Compilers & Threads

mcnp Monte Carlo Codes X-3-MCC, LANL

- Mac G5, 2.5 GHz PowerPC, OS X 10.3.9

Fortran-90	Regression tests OK ?	These runs correct ?	Wall-clock time (sec)	
			KCODE	Fixed Source
g95 -O0	Yes	Yes	535	164
g95 -O1	Yes	Yes	363	107
g95 -O2	Yes	Yes	370	113
absoft -O0	Yes	Yes	324	109
absoft -O1	Yes	Yes	352	121
absoft -O2	aborted	-	-	-
ibm xlf -O0	Yes	Yes	237	73
ibm xlf -O1	Yes	Yes	236	73
ibm xlf -O2	Yes	Yes	154	46

g95 - 0.90, absoft - 9.2, xlf - 8.1

MCNP5 - Compilers & Threads

mcnp Monte Carlo Codes X-3-MCC, LANL

- MacBook Pro, 2.16 GHz Intel Core2 Duo, OS X 10.4.8

Fortran-90	Regression tests OK ?	These runs correct ?	Threads	Wall-clock time (sec)	
				KCODE	Fixed Source
g95 -O1 (on G5), Run using Rosetta	Yes	Yes	1	727	281
g95 -O0	Yes	Yes	1	379	135
g95 -O1	Yes	Yes	1	277	87
g95 -O2	Yes	Yes	1	272	86
intel -O0 -openmp	Yes	Yes	1	256	105
			2	142	57
intel -O1 -openmp	No	Yes	1	122	55
			2	65	29
intel -O2 -openmp	No	Yes	1	113	54
			2	60	28

g95 - 0.91, intel - 9.1

MCNP and the ENDF/B-VII Cross Section Library

A. C. (Skip) Kahler, R. D. Mosteller, M. C. White

Theoretical Division & Applied Physics Division
Los Alamos National Laboratory

akahler@lanl.gov, mosteller@lanl.gov, morgan@lanl.gov

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LA-UR-07-2053

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The ENDF/B-VII Cross Section Library

- Why ENDF/B-VII; What was wrong with ENDF/B-VI?
- Processing ENDF/B-VII Neutron Files into an MCNP Library.
- Data Testing with ICSBEP Benchmarks.
- What's Improved, What Deficiencies Remain.
- Plans for Release of ENDF/B-VII Libraries for MCNP.

Why ENDF/B-VII; What was wrong with ENDF/B-VI?

- Does anyone know what ENDF/B-VI is?
  - Originally released in 1990.
    - Followed by 8 “mods” over the next 11 years (including substantial changes to ^{235}U in mods 1, 3 and 5).
    - Was frozen in 2001 following release of ENDF/B-VI.8.
  - Changes to many structural nuclide files in mods 1 & 5.
  - Changes to thermal scattering kernels in mod 2.
  - Changes to ^{1}H and ^{238}U in mod 5.
  - New photon production data for some nuclides in mod 5 and later.
  - Some revised fission product evaluations throughout, but most fp data files remain as is (including many from ENDF/B-IV).
  - Extension from 20 MeV to 150 MeV for some nuclides in mod 6.
  - Confusing nomenclature – MCNPDATA uses .60c for mod 2, uses .66c for mod 6 and uses .62c for release 8.

Why ENDF/B-VII;
What was wrong with ENDF/B-VI?

- ENDF/B-VI was significantly more complex than previous ENDF/B libraries.
  - "complex" meant physically more complete (good).
    - For example, the resolved resonance region description for ^{235}U expanded from 1 eV to 82 eV in ENDF/B-V to 10^{-5} eV to 2250 eV in ENDF/B-VI.0.
  - but "complex" also meant that greater resources (i.e., greater cost) are required to process and use this library (bad).
    - There were no dominant customers crying for ENDF/B-VI, coupled with a moribund domestic commercial reactor industry, which led to slow (or no) adoption of the new file.
      - ENDF/B-V (late 1970s/early 1980s);
      - ENDF/B-IV (early 1970s) had fast reactor support;
      - ENDF/B-III (late 1960s) had commercial reactor support.
    - Therefore, organizations that failed to adopt ENDF/B-VI are now using data that are likely to be at least 30 years old.

Why ENDF/B-VII; What was wrong with ENDF/B-VI?

- ENDF/B-VII is more complete than ENDF/B-VI.
  - 393 versus 328 neutron files;
  - 20 versus 15 thermal scattering files;
  - 3838 versus 979 radioactive decay files;
  - 163 versus 0 photonuclear files.
- Neutron files continue movement to isotopic data.
  - 390 isotopic files (carbon, vanadium and zinc are elemental).
  - 219 revised or new fission product evaluations.
    - primarily from international collaboration (WPEC-21 & 23) or developed at BNL (with KAERI collaboration).
  - have adopted existing files from other sources (e.g., JENDL-3.3) when judged appropriate.
  - revised evaluations benefit from new experimental data and from more sophisticated nuclear model codes.

Why ENDF/B-VII; What was wrong with ENDF/B-VI?

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Available online at www.sciencedirect.com

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Nuclear Data Sheets 107 (2006) 2931–3060

Nuclear Data Sheets

www.elsevier.com/locate/nds

ENDF/B-VII.0: Next Generation Evaluated Nuclear Data Library for Nuclear Science and Technology

M.B. Chadwick,[1] P. Obložinský,[2*] M. Herman,[2] N.M. Greene,[6] R.D. McKnight,[3] D.L. Smith,[3] P.G. Young,[1] R.E. MacFarlane,[1] G.M. Hale,[1] S.C. Frankle,[1] A.C. Kahler,[1,12] T. Kawano,[1] R.C. Little,[1] D.G. Madland,[1] P. Moller,[1] R.D. Mosteller,[1] P.R. Page,[1] P. Talou,[1] H. Trellue,[1] M.C. White,[1] W.B. Wilson,[1] R. Arcilla,[2] C.L. Dunford,[2] S.F. Mughabghab,[2] B. Pritychenko,[2] D. Rochman,[2] A.A. Sonzogni,[2] C.R. Lubitz,[4] T.H. Trumbull,[4] J.P. Weinman,[4] D.A. Brown,[5] D.E. Cullen,[5] D.P. Heinrichs,[5] D.P. McNabb,[5] H. Derrien,[6] M.E. Dunn,[6] N.M. Larson,[6] L.C. Leal,[6] A.D. Carlson,[7] R.C. Block,[8] J.B. Briggs,[9] E.T. Cheng,[10] H.C. Huria,[11] M.L. Zerkle,[12] K.S. Kozier,[13] A. Courcelle,[14] V. Pronyaev,[15] S.C. van der Marck[16]

[1] *Los Alamos National Laboratory, Los Alamos, NM 87545*
[2] *National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973-5000*
[3] *Argonne National Laboratory, 9700 South Cass Ave, Argonne, IL 60439-4842*
[4] *Knolls Atomic Power Laboratory, P.O. Box 1072, Schenectady, NY 12301-1072*
[5] *Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551-0808*
[6] *Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6171*
[7] *National Institute of Standards and Technology, Gaithersburg, MD 20899-8463*
[8] *Gaerttner LINAC Laboratory, Rensselaer Polytechnic Institute, Troy, NY 12180-3590*
[9] *Idaho National Laboratory, P.O. Box 1625, Idaho Falls, ID 83415-3860*
[10] *TSI Research Corp, 312 S. Cedros Ave, Solana Beach, CA 92067*
[11] *Westinghouse Electric Corp., 4350 Northern Pike, Monroeville, PA 15146*
[12] *Bettis Atomic Power Laboratory, P.O. Box 79, West Mifflin, PA 15122*
[13] *Atomic Energy of Canada Ltd., Chalk River, ON K0J 1J0, Canada*
[14] *Centre d'Études Nucléaires de Cadarache, F-13108 Saint-Paul lèz Durance, Cedex, France*
[15] *Institute for Physics and Power Engineering, Ploschad Bondarenko 1, 249 020 Obninsk, Russia and*
[16] *Nuclear Research and Consultancy Group, P.O. Box 25, NL-1755 ZG Petten, The Netherlands*

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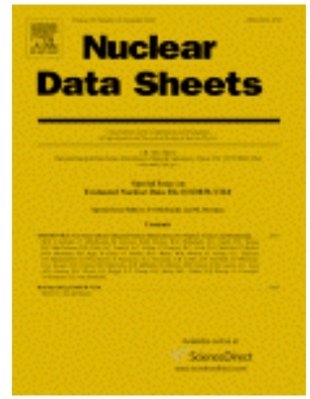


- The ENDF/B-VII.0 cross section library may be downloaded from Brookhaven National Laboratory's National Nuclear Data Center (NNDC), http://www.nndc.bnl.gov/exfor7/endf00.htm.

Processing ENDF/B-VII Neutron Files into an MCNP Library

- The Los Alamos NJOY Nuclear Data Processing Program converts an ENDF-formatted file into an MCNP ACE file.
  - The base version of NJOY (currently NJOY99) is available from ORNL (RSICC) or the Nuclear Energy Agency;
  - Updates are available at http://t2.lanl.gov/codes/njoy99/index.html.
    - includes machine and compiler guidance plus sample problem I/O.
  - User information is available at http://www.nea.fr/lists/njoy.html or at http://www-rsicc.ornl.gov/ENOTE/enotnjoy.html.

- For each ENDF evaluation NJOY can create:
  - a unique, doppler broadened, linearly interpolable, unionized cross section mesh for all cross sections for that material;
  - angular distribution probability functions;
  - secondary energy spectra.

Processing ENDF/B-VII Neutron Files into an MCNP Library

- The most commonly used NJOY modules include:
  - MODER: ascii to binary conversion for efficient I/O (optional).
  - RECONR: resonance reconstruction, cross section linearization and energy mesh unionization at zero degrees.
  - BROADR: doppler broadening to User specified temperature, including energy mesh adjustment to maintain user specified linear-linear interpolation accuracy.
  - UNRESR: unresolved resonance processing (to support HEATR).
  - HEATR: heating and energy damage calculations (a standard part of MCNP ACE files, but not needed for criticality calculations).
  - PURR: unresolved resonance processing (probability tables).
  - THERMR: thermal scattering kernel processing (maybe in conjunction with the LEAPR module).
  - ACER: create an MCNP continuous energy (.c) and thermal kernel (.t) library files.

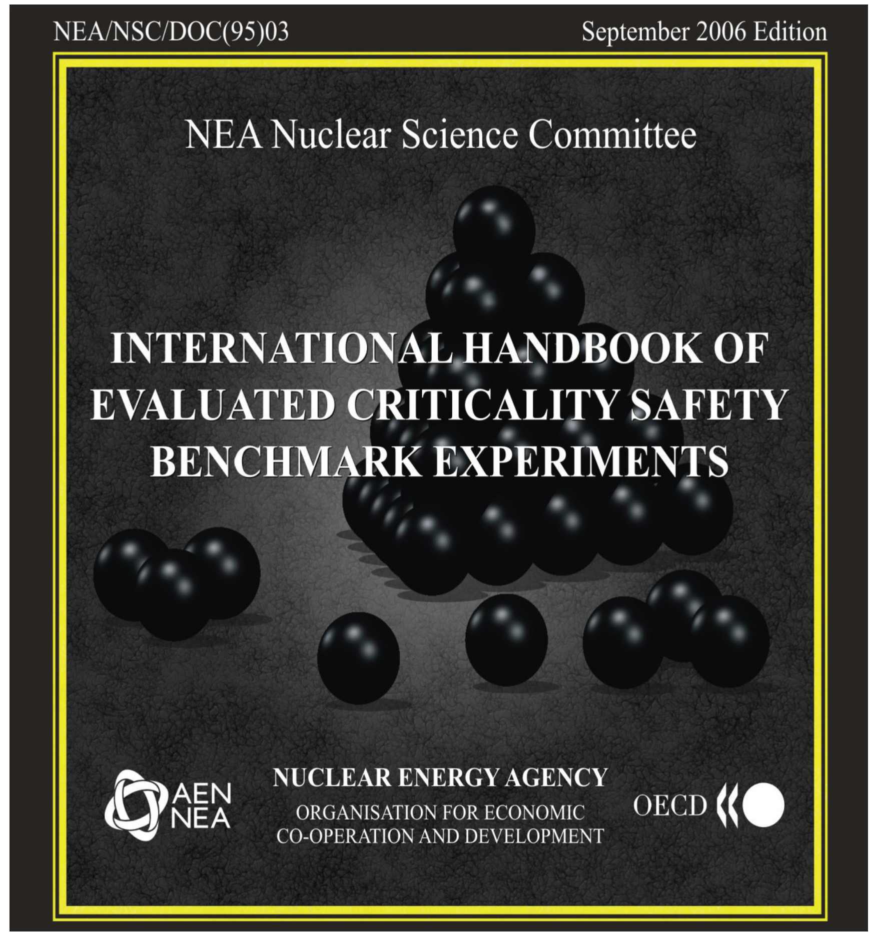
Processing ENDF/B-VII Neutron Files into an MCNP Library

- Independently compiled versions of NJOY (99.162 at Brookhaven National Laboratory's National Nuclear Data Center (NNDC) or 99.167 at LANL) have successfully created ACE-formatted files for all 393 ENDF/B-VII.0 neutron files.

- The ENDF/B-VII.0 cross section library may be obtained at http://www.nndc.bnl.gov/exfor7/endf00.htm.

Data Testing with ICSBEP Benchmarks

- ICSBEP = International Criticality Safety Benchmark Evaluation Project.
- Responsible for the content of the International Handbook of Evaluated Criticality Safety Benchmark Experiments.
- The Handbook is updated and re-issued annually in the Fall.
  - For 2006 there are 442 evaluations with 3955 configurations.
- http://icsbep.inel.gov/



Data Testing with ICSBEP Benchmarks

- The Handbook has distinct categories for fissile material, physical form of that material and spectrum.
  - Fissile material categories include
    - HEU: > 60 wt.% ^{235}U;
    - IEU: 10 wt.% < ^{235}U < 60 wt.%;
    - LEU: < 10 wt.% ^{235}U;
    - Pu: mostly ^{239}Pu, some configurations with > 40 at.% ^{240}Pu;
    - U233:
    - Mixed Pu-U:
    - Special Isotopes (e.g. ^{237}Np).
  - Categories for the physical form of the fissile material include:
    - Metal;
    - Compound (e.g. UO_2);
    - Solution (mostly nitrates and fluorides).

Data Testing with ICSBEP Benchmarks

- The Handbook has distinct categories for fissile material, physical form of that material and spectrum (con't).
  - Fission spectrum categories include:
    - Fast: > 50% of the fissions occur above 100 keV;
    - Intermediate: > 50% of the fissions occur between 0.625 eV & 100 keV.
    - Thermal: > 50% of the fission occur below 0.625 eV;
    - Mixed: < 50% of the fissions occur in each category.

  - In recent years the scope of the Handbook has expanded to include radiation transport measurements applicable to Criticality Alarm & Shielding Benchmarks as well as Fundamental Physics Measurements.

Data Testing with ICSBEP Benchmarks

- ICSBEP Nomenclature
  - A given benchmark is identified by its fissile material, its physical form, the dominant fission spectrum category and a sequence number.
    - Examples
      - HEU-MET-FAST-001: Godiva
      - HEU-MET-FAST-028: Flattop-28
      - PU-MET-FAST-001: Jezebel
      - PU-MET-FAST-006: Thor
      - U233-MET-FAST-001: Jezebel-233
- Although not a formal category, many benchmarks include metallic and/or non-hydrogenous reflectors.

Data Testing with ICSBEP Benchmarks

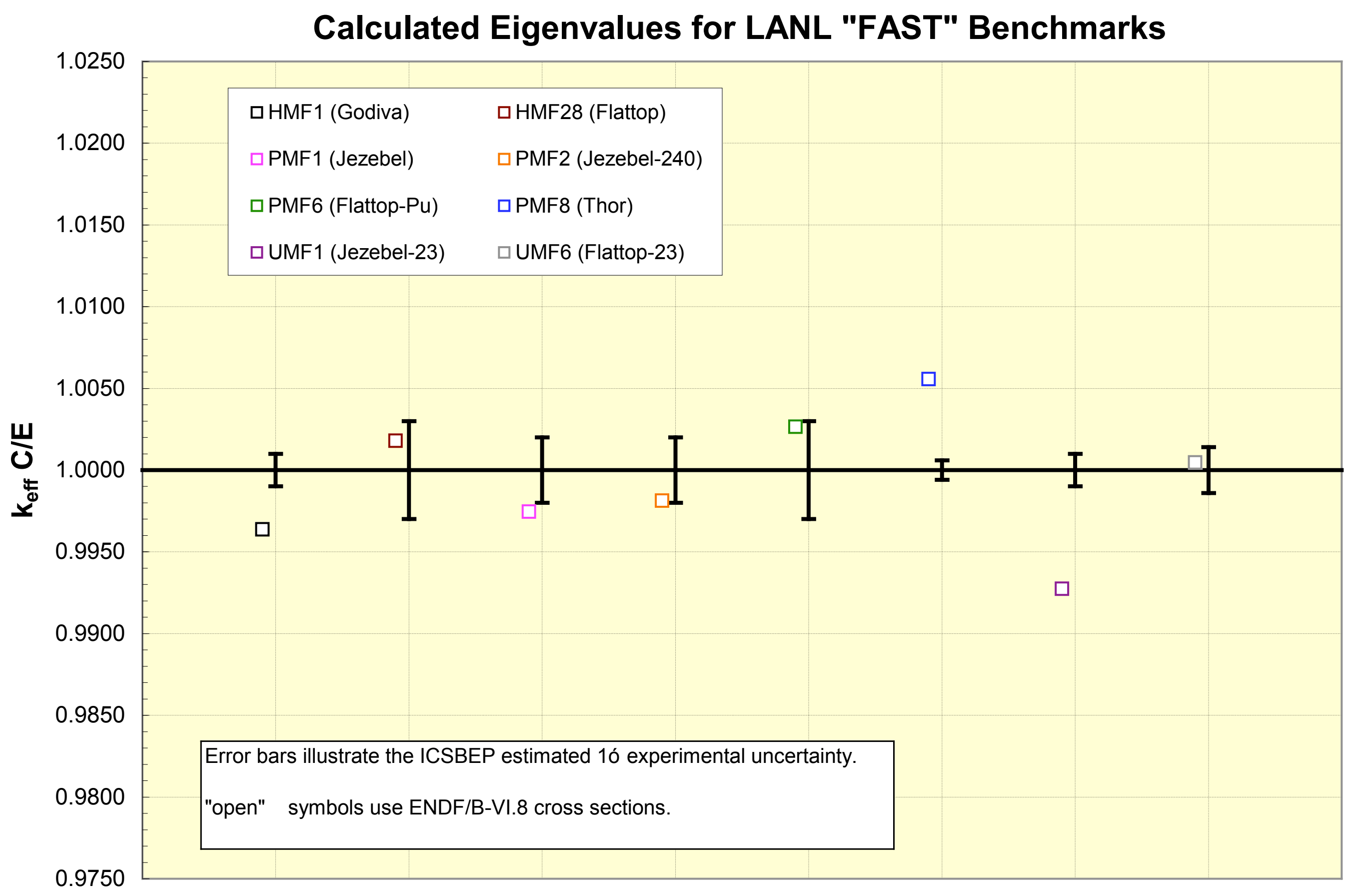
- LANL has developed MCNP models for hundreds of the ICSBEP benchmarks and performed critical eigenvalue calculations for them with various cross section data sets.

- Comparison of calculated critical eigenvalues illustrate areas of improvement and point to where future efforts to improve fundamental nuclear data are needed.

- Back to the original question –
  - why ENDF/B-VII, what was wrong with ENDF/B-VI?

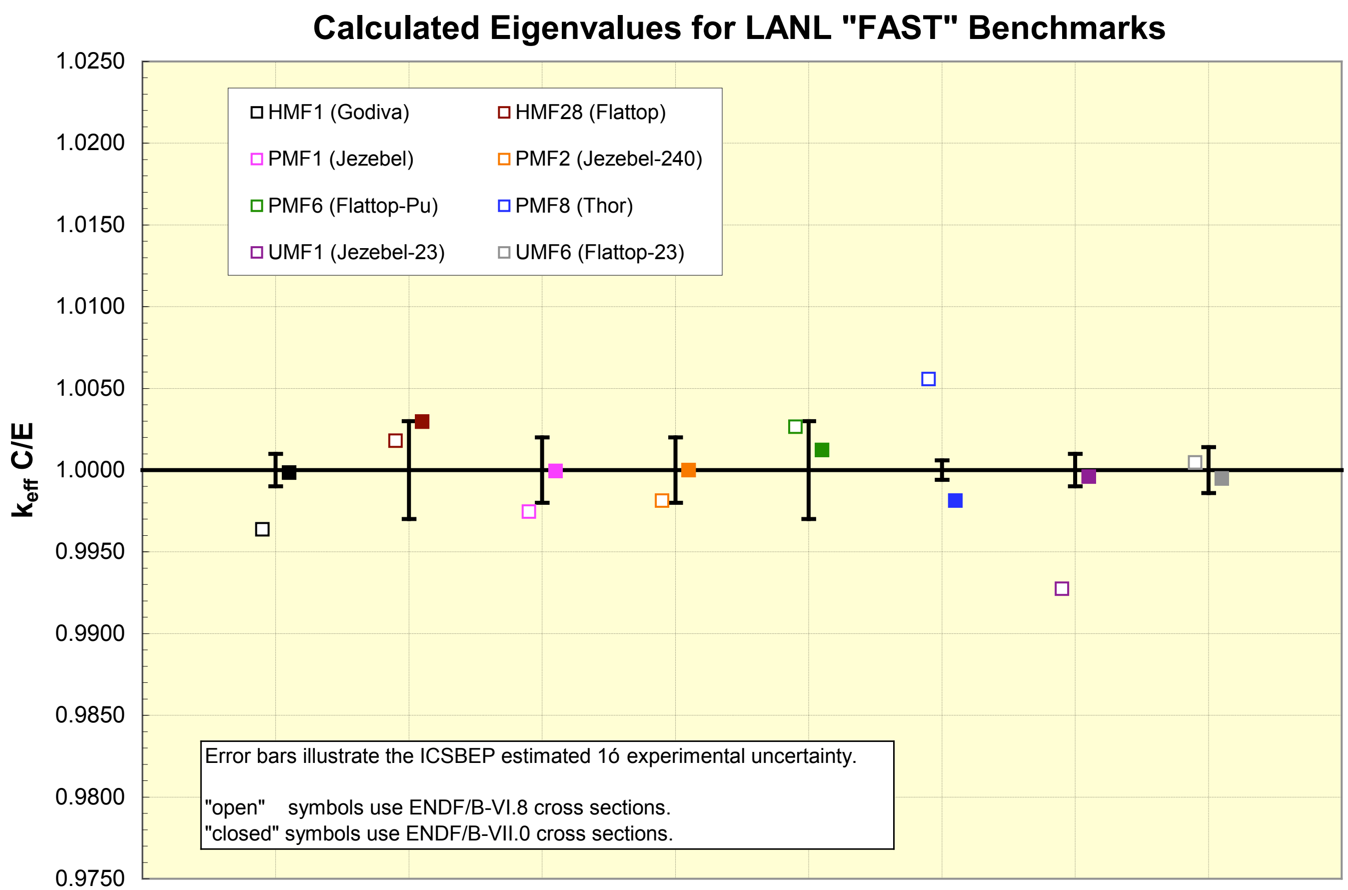
- Representative results follow:

Data Testing with ICSBEP Benchmarks



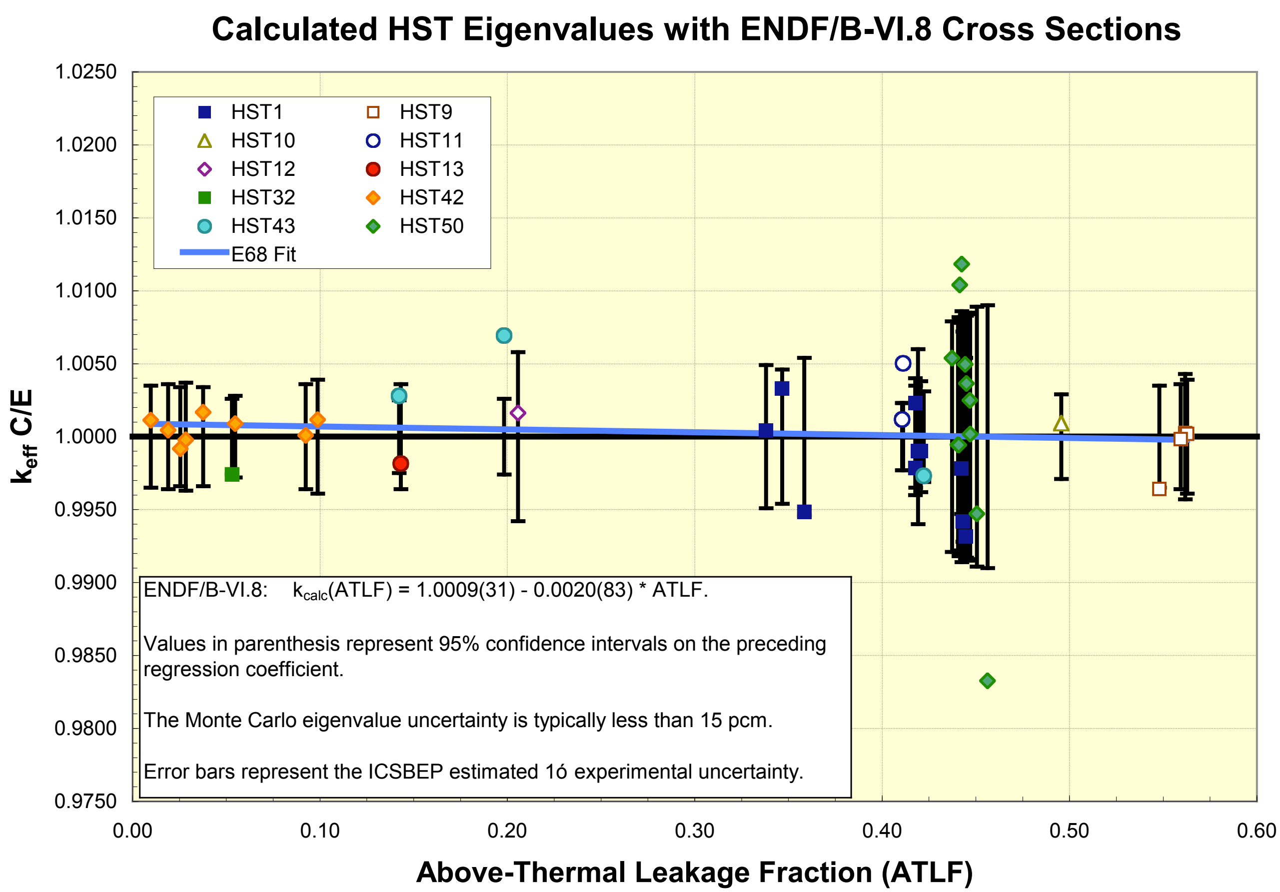
- ENDF/B-VI.8 eigenvalues for Historical LANL "Fast" Benchmarks.
- Eigenvalues are biased low by several hundred pcm for all bare systems.
- A reflector bias is readily observed.

Data Testing with ICSBEP Benchmarks



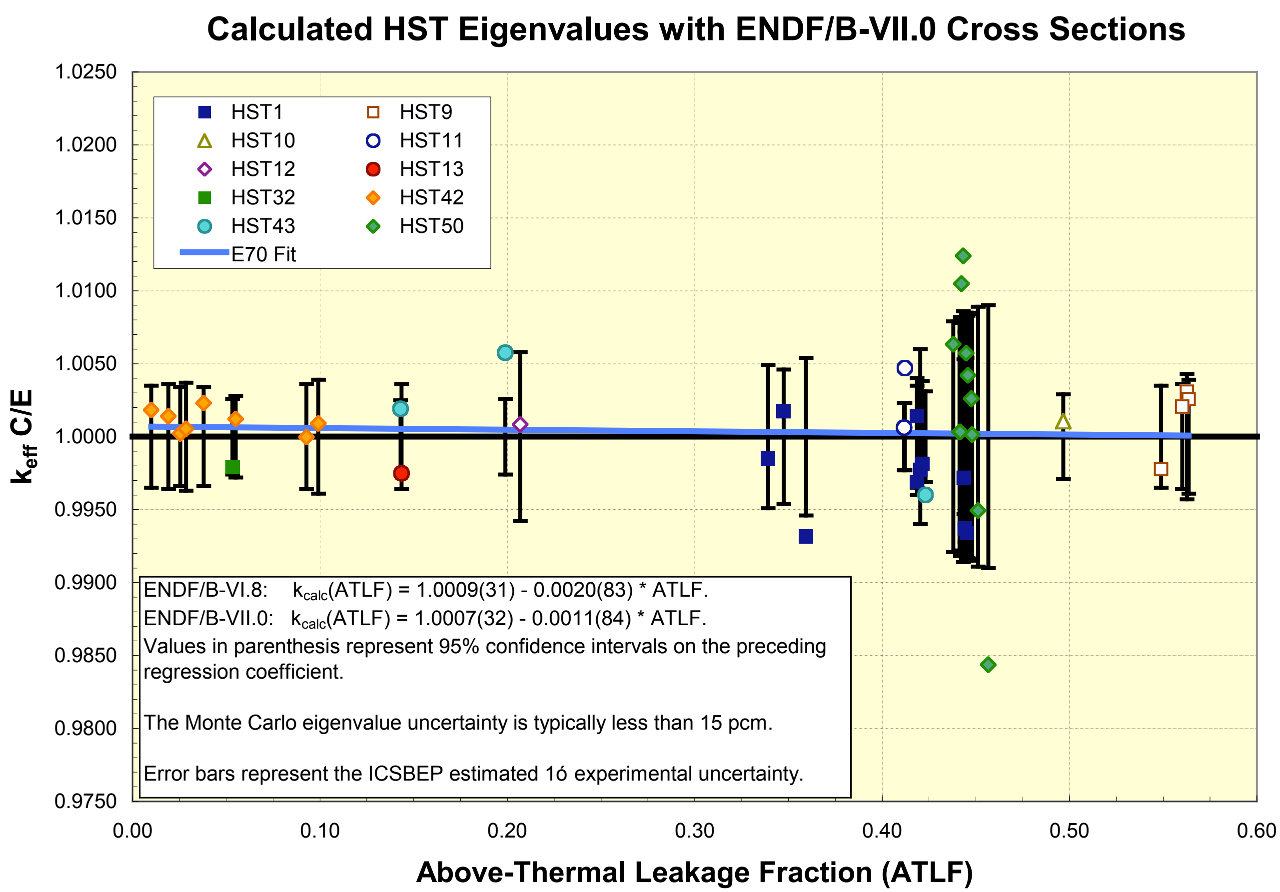
- An ENDF/B-VII.0 success story.
- Calculated eigenvalues are significantly closer to unity than those obtained with ENDF/B-VI.8 cross sections.
- The reflector bias is virtually eliminated.

Data Testing with ICSBEP Benchmarks



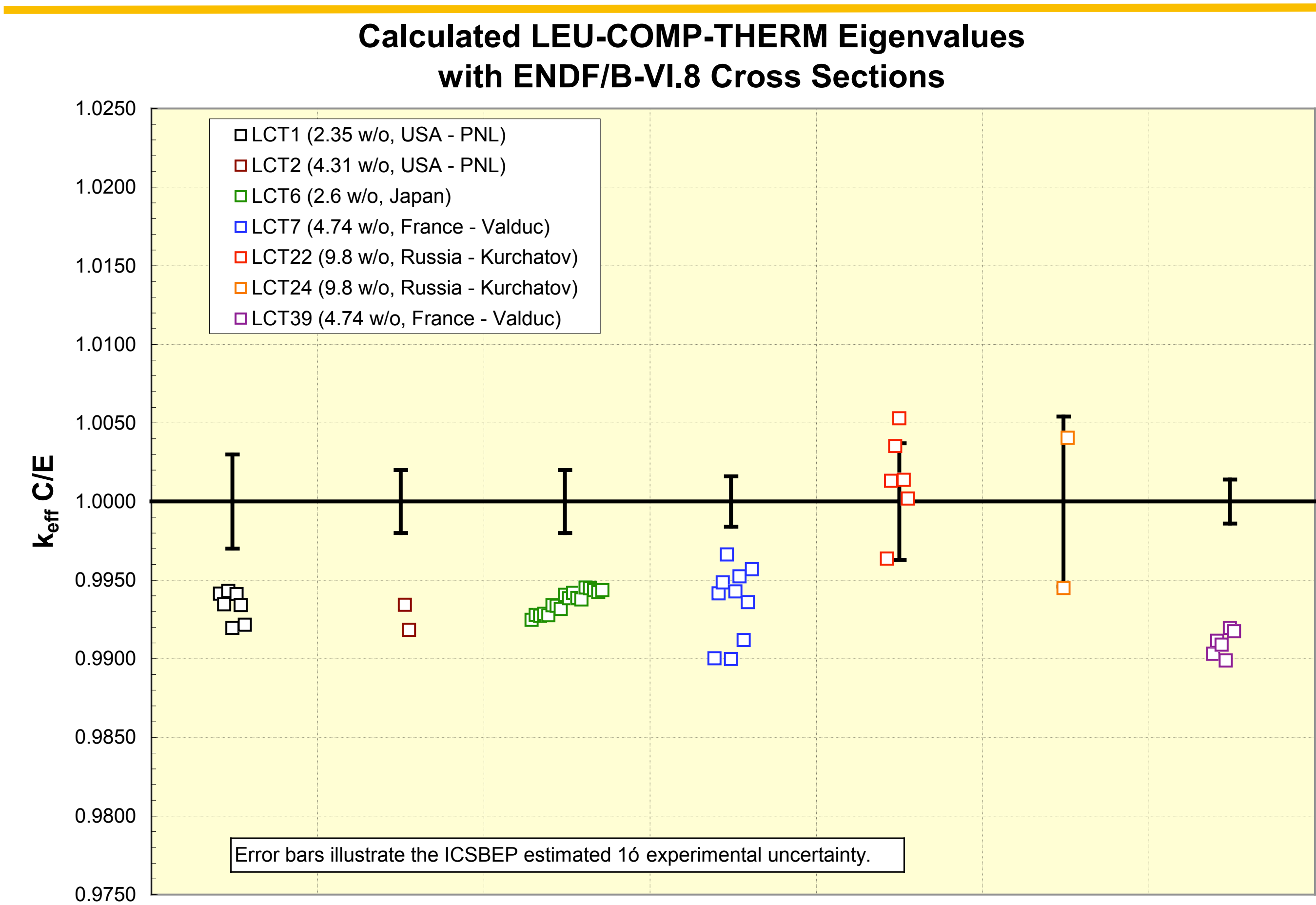
- Calculated eigenvalues for uranium solutions are an ENDF/B-VI success story.
- Eigenvalue biases and trends observed in previous ENDF/B cross sections were eliminated starting with ENDF/B-VI.3.

Data Testing with ICSBEP Benchmarks



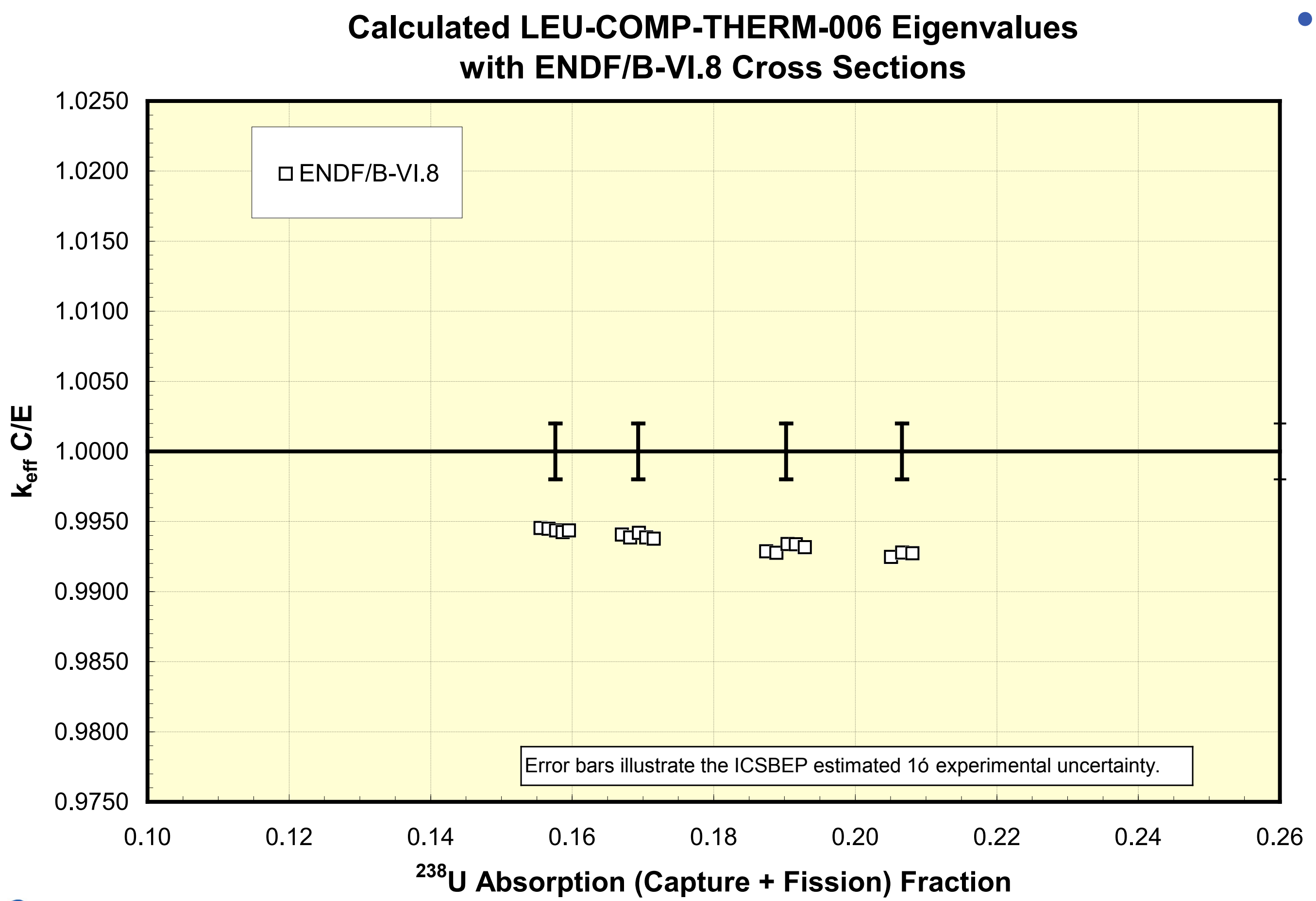
- Results with ENDF/B-VII.0 remain excellent, despite changes in the underlying $^{235,238}U$, ^{1}H and ^{16}O cross sections.

Data Testing with ICSBEP Benchmarks



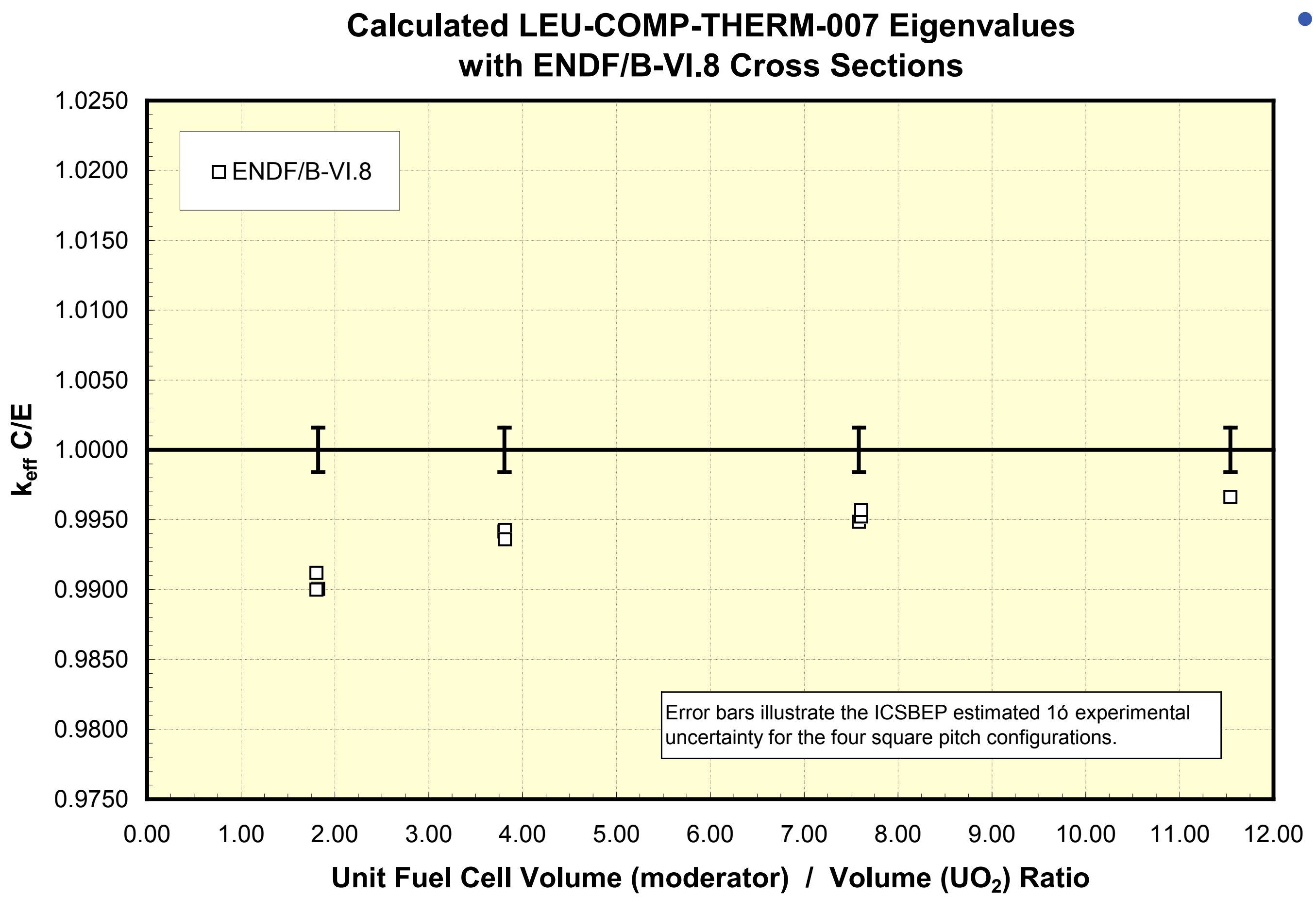
- ENDF/B-VI based LEU-COMP-THERM calculated eigen-values are low and exhibit trends with ^{238}U absorption frac-tion and funda-mental lattice parameters.
- These are long-standing, histor-ical deficiencies inherited from ENDF/B-V (and earlier).

Data Testing with ICSBEP Benchmarks



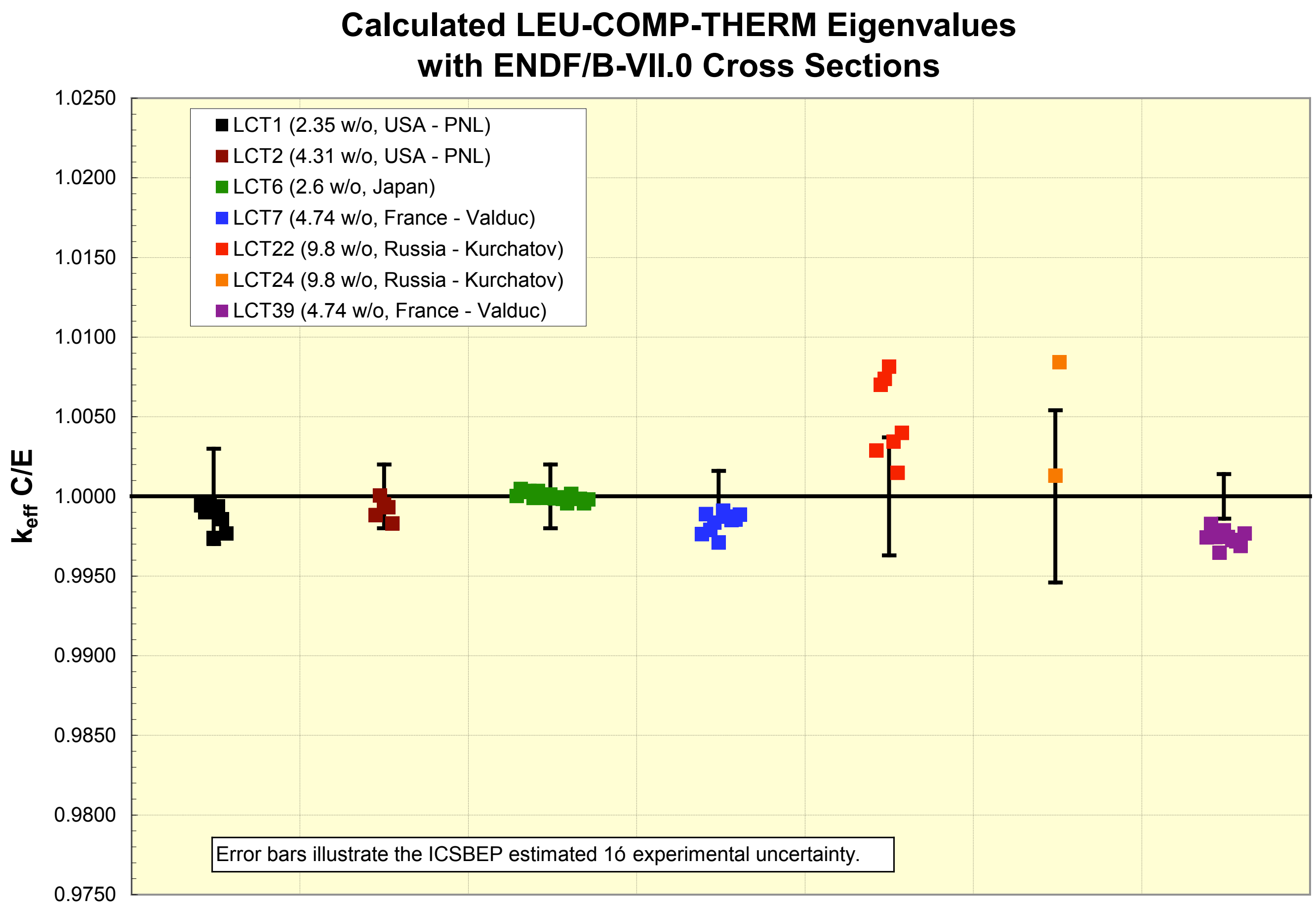
- LEU-COMP-THERM-006 (Japan) provides an excellent example of the ENDF/B-VI.8 calculated eigenvalue trend as a function of ^{238}U absorption.

Data Testing with ICSBEP Benchmarks



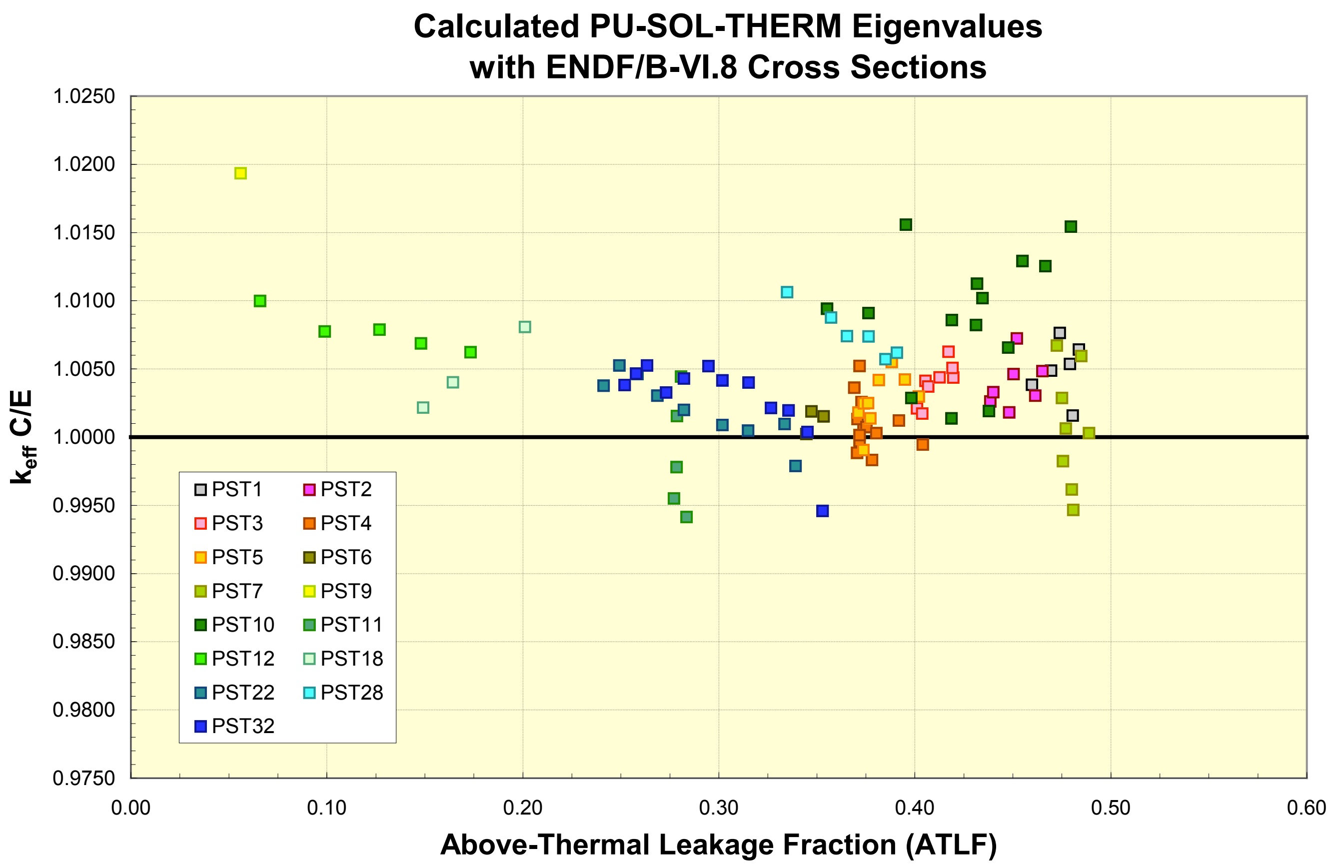
- LEU-COMP-THERM-007 (France) provides an excellent example of the ENDF/B-VI.8 calculated eigenvalue trend as a function of H/U ratio (lattice pitch).

Data Testing with ICSBEP Benchmarks



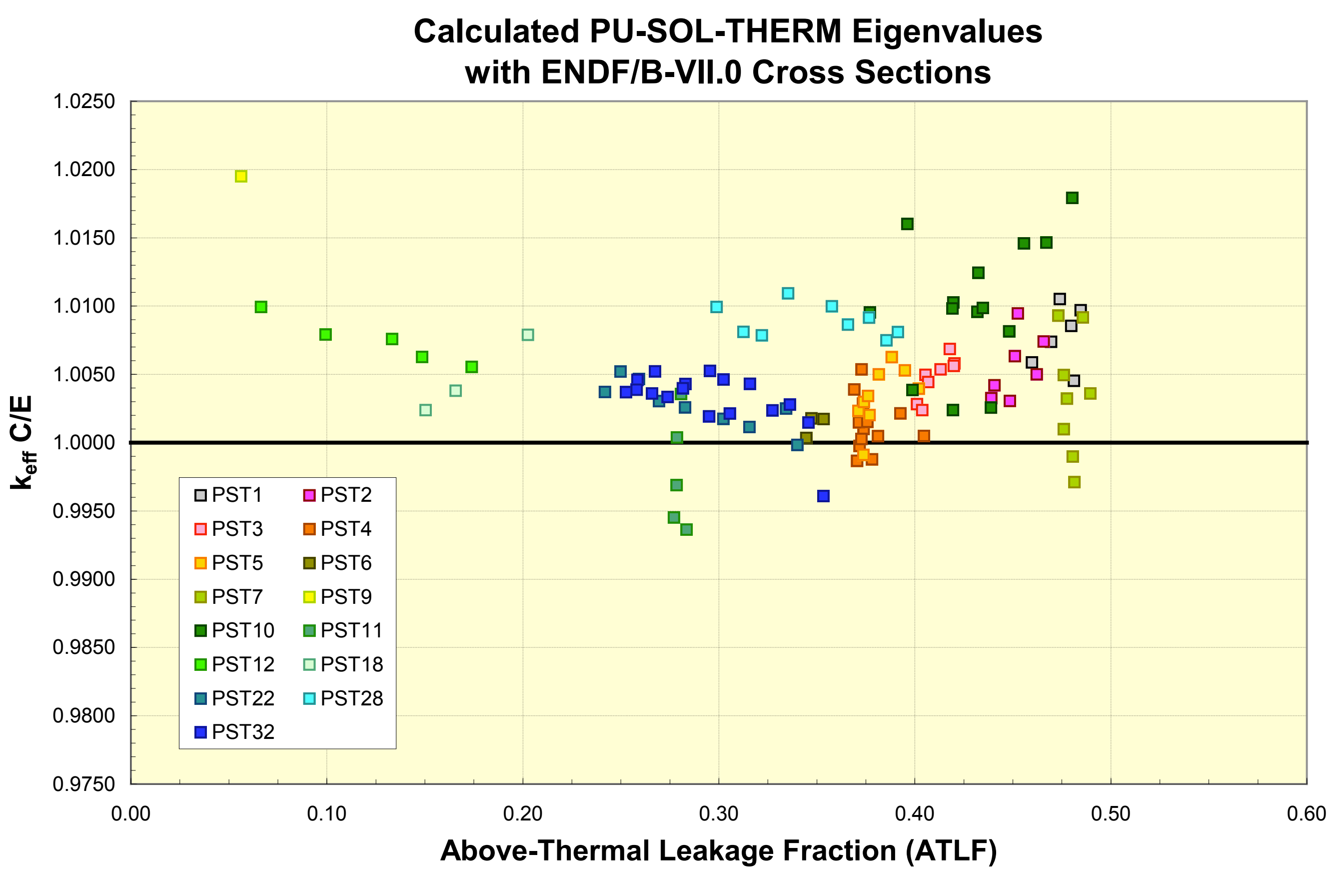
- ENDF/B-VII.0 based LEU-COMP-THERM calculated eigen-values are signif-icantly closer to unity.

Data Testing with ICSBEP Benchmarks



- ENDF/B-VI.8 Based Pu Solution System Calculated Eigenvalues are Biased High.
- There are no obvious trends in these eigen-values when correlated against various system parameters (e.g. ^{240}Pu at. %, leakage, ^{1}H absorption frac-tion, thermal fission fraction, Pu concentration, …).

Data Testing with ICSBEP Benchmarks



- There has been little work on thermal Pu cross sections for ENDF/B-VII, hence the calculated eigenvalue deficiency remains.

Data Testing with ICSBEP Benchmarks

- Acknowledgements
- Preliminary ACE formatted cross section files derived from ENDF/B-VII.0 neutron and thermal scattering kernel files used in these calculations were processed with NJOY99.167 by R. E. MacFarlane. Bob has been and continues to be a significant contributor to LANL's ENDF/B-VII data testing effort.
- ENDF/B-VI.8 results were obtained using publicly available MCNPDATA files (.66c and .62c and associated ENDF/B-VI.2 thermal scattering kernels).

Data Testing with ICSBEP Benchmarks

- And now for the rest of the story …

ENDF70 - ACE Data Based On ENDF/B-VI.0

- Expected Release in Late Summer (On Track!)
- Initial release will include continuous-energy neutron and photon data and S(alpha,beta) tables
  - Continuous-energy neutron library will include all 393 tables
    - Initial indications are promising that ENDF/B-VII.0 is “complete”
    - Data at 293.6, 600, 900, 1200 & 2500 K
      - Doppler broadening to other temperatures via MAKXSF
  - All 20 thermal scattering tables
    - Data at all evaluated temperatures
  - MCPLIB04 includes photoatomic data for 100 elements
    - No changes were made to the photon data between VI.8 and VII.0
- Incident charged particle and photonuclear tables will be released “at a later date”

Verification, Verification, Verification
The ENDF66 Success Story

- Zero (0!) bug reports since ENDF66 was released
- Our team consider themselves to be master data breakers
  - We have stressed the data, NJOY, MCNP and PARTISN to their limits and helped make their use more robust
  - Our friendly users add even more stress to the system
  - Most of our time on this project will be spent on the 80/20 rule
    - And it's actually more like 95/5
- It's All About Verification
  - A wide variety of tools are employed to check the data "six-ways-from-Sunday"
- ENDF70 is in the process of undergoing similar QA

Benchmark Anomalies and Persistent Problems in Nuclear-Data Testing for ENDF/B-VII.0

Russell D. Mosteller

Applied Physics Division
Los Alamos National Laboratory
mosteller@ lanl.gov

Presented at the MCNP Workshop at MCD + SNA 2007
Monterey, CA April 15, 2007

OVERVIEW OF PRESENTATION

Identification of nuclear data libraries and details of calculations

Cases and results (all input specifications are taken from *International Handbook of Evaluated Criticality Safety Benchmark Experiments*)

- Zeus HEU-graphite benchmarks (^{235}U in unresolved resonance range)
- Unmoderated Zeus HEU benchmark (copper in fast range)
- Neptunium sphere benchmark (^{237}Np in fast range)
- Benchmarks of HEU nitrate solutions in heavy water (angular scattering distributions for ^{2}H)
- MOX lattice benchmarks (^{239}Pu in thermal range)
- Plutonium nitrate solution benchmarks (^{239}Pu in thermal range)
- HEU nitrate solution benchmark with Cd (^{113}Cd in thermal range)

Conclusions

NUCLEAR DATA LIBRARIES

Evaluated Nuclear Data File VII, Release 0 (ENDF/B-VII.0)

Evaluated Nuclear Data File VI, Release 8 (ENDF/B-VI)

Evaluated Nuclear Data File V (ENDF/B-V)

Japanese Evaluated Nuclear Data Library, version 3.3 (JENDL-3.3)

Joint Evaluated Fission and Fusion file, version 3.1 (JEFF-3.1)

MCNP5 CALCULATIONS

Each calculation employed at least 550 generations with 10,000 neutrons per generation

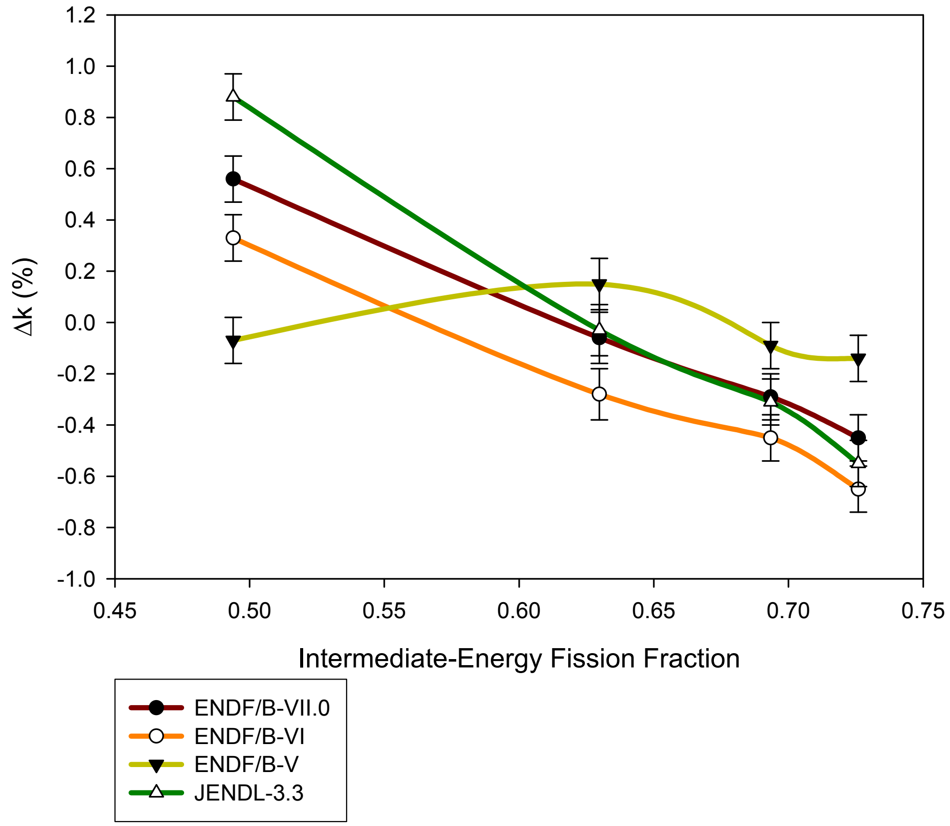
Results from first 50 generations were excluded from the statistics

Results therefore are based on at least 5,000,000 active histories for each case

CRITICALITY BENCHMARKS

Name	Spectrum	*Handbook* ID	Description
Zeus-1	Intermediate	HEU-MET-INTER-006, case 1	HEU platters moderated by graphite and reflected by copper
Zeus-2	Intermediate	HEU-MET-INTER-006, case 2	HEU platters moderated by graphite and reflected by copper
Zeus-3	Intermediate	HEU-MET-INTER-006, case 3	HEU platters moderated by graphite and reflected by copper
Zeus-4	Intermediate	HEU-MET-INTER-006, case 4	HEU platters moderated by graphite and reflected by copper
Unmod Zeus	Fast	HEU-MET-FAST-073	HEU platters reflected by copper
Np Sphere	Fast	SPEC-MET-FAST-008	Neptunium sphere reflected by HEU shells
HST-4	Intermediate	HEU-SOL-THERM-004, cases 1-2	Reflected spheres of HEU solution in heavy water
HST-4	Thermal	HEU-SOL-THERM-004, cases 3-6	Reflected spheres of HEU solution in heavy water
HST-20	Thermal	HEU-SOL-THERM-020, cases 1-5	Unreflected cylinders of HEU solution in heavy water
PNL-30	Thermal	MIX-COMP-THERM-002, case 30	Lattice of 469 MOX pins (2 wt.% PuO_2) in water (1.7 PPM)
PNL-31	Thermal	MIX-COMP-THERM-002, case 31	Lattice of 761 MOX pins (2 wt.% PuO_2) in water (687.9 PPM)
PNL-32	Thermal	MIX-COMP-THERM-002, case 32	Lattice of 195 MOX pins (2 wt.% PuO_2) in water (0.9 PPM)
PNL-33	Thermal	MIX-COMP-THERM-002, case 33	Lattice of 761 MOX pins (2 wt.% PuO_2) in water (1090.4 PPM)
PNL-34	Thermal	MIX-COMP-THERM-002, case 34	Lattice of 161 MOX pins (2 wt.% PuO_2) in water (1.6 PPM)
PNL-35	Thermal	MIX-COMP-THERM-002, case 35	Lattice of 689 MOX pins (2 wt.% PuO_2) in water (767.2 PPM)
PNL-1	Thermal	PU-SOL-THERM-021, case 7	Unreflected 14-inch sphere of plutonium nitrate solution
PNL-3	Thermal	PU-SOL-THERM-011, case 18-1	Unreflected 18-inch sphere of plutonium nitrate solution
PNL-4	Thermal	PU-SOL-THERM-011, case 18-6	Unreflected 18-inch sphere of plutonium nitrate solution
PNL-5	Thermal	PU-SOL-THERM-011, case 16-5	Unreflected 16-inch sphere of plutonium nitrate solution
PNL-6	Thermal	PU-SOL-THERM-021, case 3	Unreflected 15.2-inch sphere of plutonium nitrate solution
PNL-8	Thermal	PU-SOL-THERM-021, case 2	Unreflected 15.2-inch sphere of plutonium nitrate solution
PST-9	Thermal	PU-SOL-THERM-009, case 3a	Unreflected 48-inch sphere of plutonium nitrate solution
HST-49c20	Thermal	HEU-SOL-THERM-049, case 20	Reflected cylinder of HEU nitrate solution with Cd

ZEUS HEU-GRAPHITE BENCHMARKS



⇒ Cross sections for ^{235}U in the unresolved resonance region should be re-examined

UNMODERATED ZEUS BENCHMARK

Source	k_{eff}	Δk
Benchmark	1.0004 ± 0.0016	—
ENDF/B-VII.0	1.0116 ± 0.0003	0.0112 ± 0.0016
ENDF/B-VI	1.0082 ± 0.0003	0.0078 ± 0.0016
JENDL-3.3	1.0242 ± 0.0003	0.0238 ± 0.0016

$|\Delta k| > 4\sigma$

Benchmark contains no moderator and therefore has a fast spectrum

All three calculated results differ from the benchmark value for k_{eff} by more than 4 standard deviations

Results for k_{eff} with ENDF/B-V Cross Sections for Copper

Source	k_{eff}	Δk
Benchmark	1.0004 ± 0.0016	—
ENDF/B-VII.0	1.0001 ± 0.0003	-0.0003 ± 0.0016
ENDF/B-VI	0.9971 ± 0.0003	-0.0033 ± 0.0016
JENDL-3.3	1.0001 ± 0.0003	-0.0003 ± 0.0016

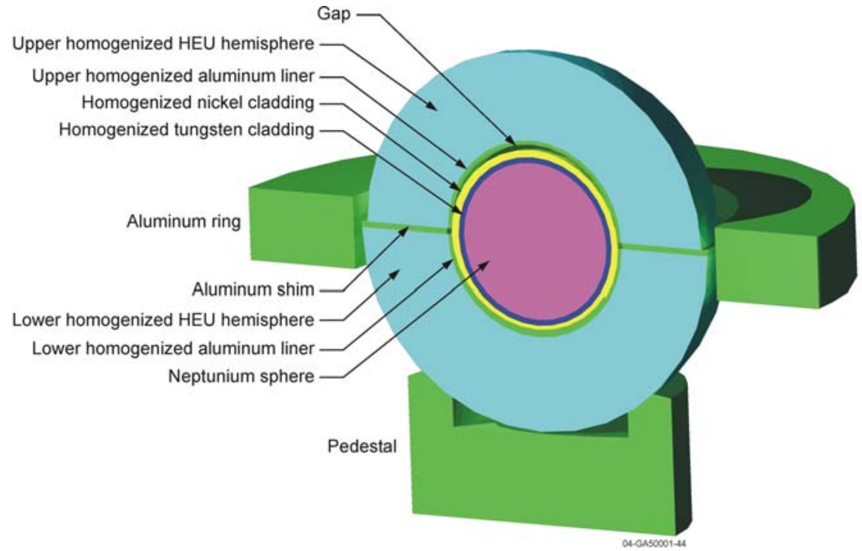
$|\Delta k| > 2\sigma$

Both JENDL-3.3 and ENDF/B-VII.0 now produce results for k_{eff} that are within a single standard deviation of the experimental value

Differences between ENDF/B-V and ENDF/B-VII.0 Cu cross sections have little net reactivity impact on previous Zeus benchmarks, which have intermediate spectra

⇒ Fast cross sections for Cu should be reviewed

NEPTUNIUM SPHERE REFLECTED BY HEU



Benchmark k_{eff}	Calculated k_{eff}		
	ENDF/B-VII.0	ENDF/B-VI	JENDL-3.3
1.0019 ± 0.0036	0.9951 ± 0.0003	0.9889 ± 0.0002	0.9967 ± 0.0002

$\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

⇒ Fast cross sections for ^{237}Np should be reviewed

HEAVY-WATER SOLUTIONS

Case	Benchmark k_{eff}	Calculated k_{eff}		
		ENDF/B-VII.0 + JENDL-3.3 ^{2}H	ENDF/B-VII.0	JENDL-3.3
Reflected Spheres (HEU-SOL-THERM-004)				
1	1.0000 ± 0.0033	0.9967 ± 0.0004	0.9847 ± 0.0004	0.9918 ± 0.0004
2	1.0000 ± 0.0036	0.9919 ± 0.0004	0.9815 ± 0.0004	0.9873 ± 0.0004
3	1.0000 ± 0.0039	0.9985 ± 0.0004	0.9883 ± 0.0004	0.9944 ± 0.0004
4	1.0000 ± 0.0046	1.0012 ± 0.0004	0.9904 ± 0.0004	0.9971 ± 0.0004
5	1.0000 ± 0.0052	0.9994 ± 0.0005	0.9891 ± 0.0004	0.9956 ± 0.0004
6	1.0000 ± 0.0059	0.9959 ± 0.0004	0.9854 ± 0.0004	0.9913 ± 0.0004
Unreflected Cylinders (HEU-SOL-THERM-020)				
1	0.9966 ± 0.0116	1.0039 ± 0.0005	0.9932 ± 0.0005	1.0006 ± 0.0005
2	0.9956 ± 0.0093	1.0105 ± 0.0005	0.9983 ± 0.0005	1.0066 ± 0.0005
3	0.9957 ± 0.0079	1.0185 ± 0.0005	1.0070 ± 0.0005	1.0149 ± 0.0005
4	0.9955 ± 0.0078	1.0162 ± 0.0005	1.0048 ± 0.0005	1.0160 ± 0.0005
5	0.9959 ± 0.0077	1.0234 ± 0.0005	1.0131 ± 0.0005	1.0167 ± 0.0005

$\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

PNL MOX Lattices

Case	Pitch (cm)	Soluble Boron (PPM)	Benchmark k_{eff}	Calculated k_{eff}		
				ENDF/B-VII.0	ENDF/B-VI	JENDL-3.3
PNL-30	1.77800	1.7	1.0010 ± 0.0059	1.0019 ± 0.0003	0.9933 ± 0.0003	0.9987 ± 0.0003
PNL-31	1.77800	687.9	1.0009 ± 0.0045	1.0028 ± 0.0003	0.9960 ± 0.0004	1.0008 ± 0.0004
PNL-32	2.20914	0.9	1.0024 ± 0.0029	1.0035 ± 0.0003	0.9965 ± 0.0004	1.0018 ± 0.0003
PNL-33	2.20914	1090.4	1.0024 ± 0.0021	1.0072 ± 0.0003	1.0029 ± 0.0003	1.0069 ± 0.0003
PNL-34	2.51447	1.6	1.0038 ± 0.0022	1.0041 ± 0.0003	0.9989 ± 0.0003	1.0033 ± 0.0003
PNL-35	2.51447	767.2	1.0029 ± 0.0024	1.0069 ± 0.0003	1.0031 ± 0.0003	1.0062 ± 0.0004

$\sigma < |\Delta k| \leq 2\sigma$

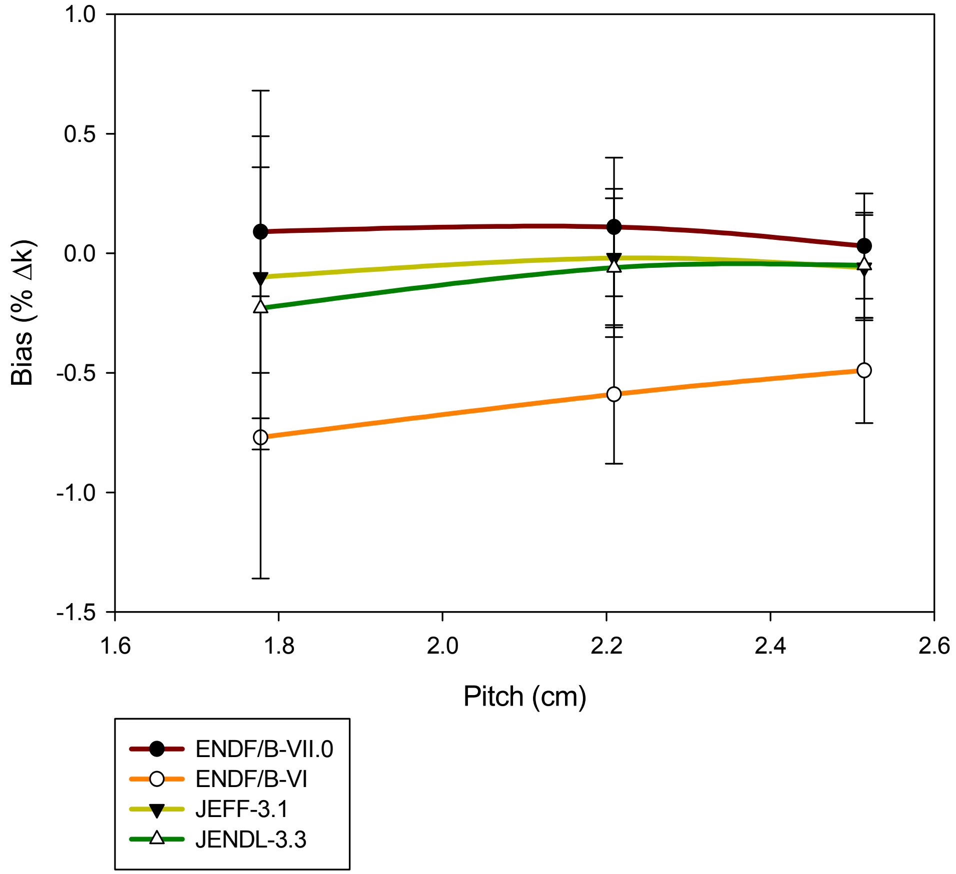
$|\Delta k| > 2\sigma$

Overall, ENDF/B-VII.0 produces best results

None of the ENDF/B-VII.0 values for k_{eff} are lower than the corresponding mean benchmark value, but two are higher by more than 1 standard deviation

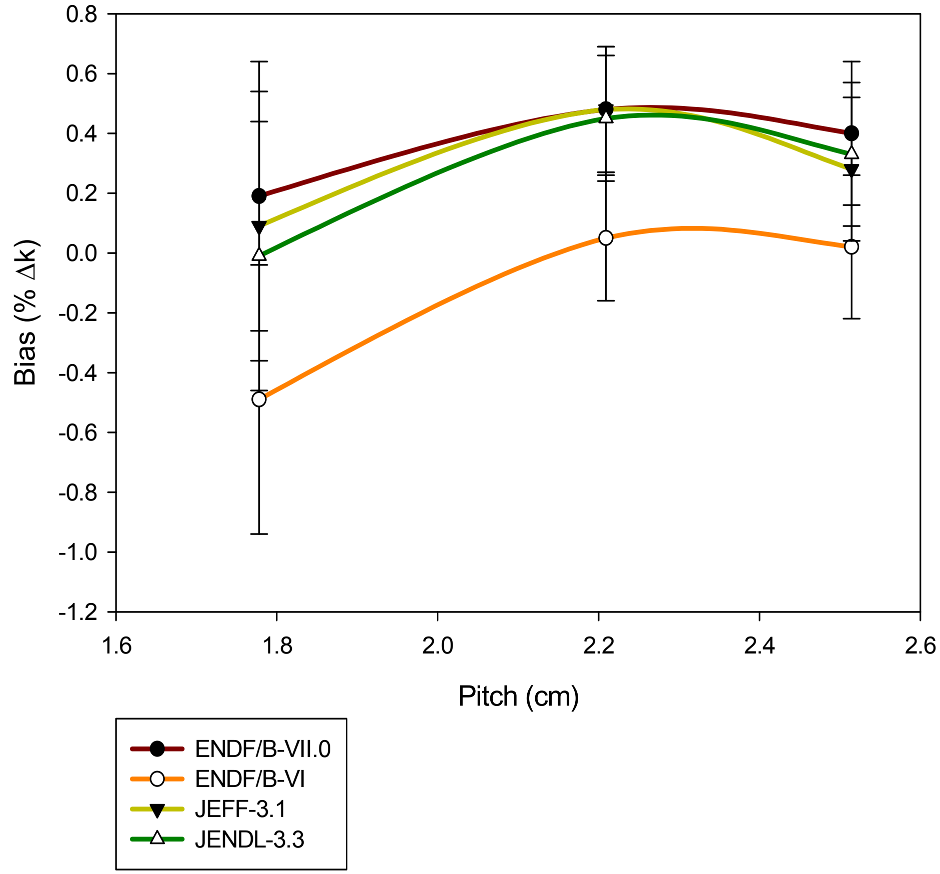
All 3 libraries produce different shapes for slightly and highly borated cases

Slightly Borated PNL MOX Lattices



ENDF/B-VII.0 produces significant improvement relative to ENDF/B-VI

Highly Borated PNL MOX Lattices



⇒ Thermal cross sections for ^{239}Pu probably should be reviewed

Unreflected Spheres of Plutonium-Nitrate Solutions

Case	H / ^{239}Pu Atom Radio	Benchmark k_{eff}	Calculated k_{eff}		
			ENDF/B-VII.0	ENDF/B-VI	JENDL-3.3
PNL-6	131.83	1.0000 ± 0.0065	1.0040 ± 0.0005	1.0029 ± 0.0005	1.0070 ± 0.0004
PNL-5	574.52	1.0000 ± 0.0052	1.0066 ± 0.0004	1.0058 ± 0.0004	1.0098 ± 0.0004
PNL-1	701.70	1.0000 ± 0.0032	1.0066 ± 0.0004	1.0066 ± 0.0004	1.0101 ± 0.0004
PNL-8	797.62	1.0000 ± 0.0032	1.0052 ± 0.0004	1.0060 ± 0.0004	1.0101 ± 0.0004
PNL-4	907.13	1.0000 ± 0.0052	1.0002 ± 0.0004	1.0012 ± 0.0004	1.0043 ± 0.0004
PNL-3	1207.8	1.0000 ± 0.0052	0.9950 ± 0.0004	0.9954 ± 0.0004	0.9985 ± 0.0004
PST-9	2806.8	1.0003 ± 0.0033	1.0189 ± 0.0002	1.0190 ± 0.0002	1.0226 ± 0.0002

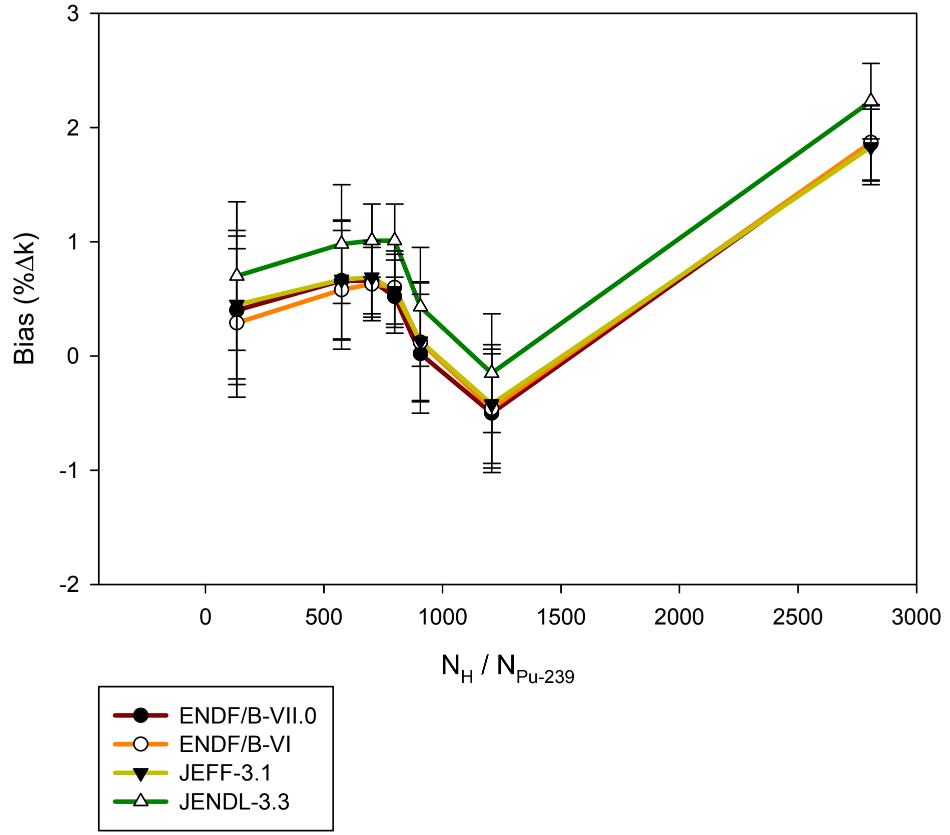
$\sigma < |\Delta k| \leq 2\sigma$ $|\Delta k| > 2\sigma$

ENDF/B-VII.0 results are very similar to those from ENDF/B-VI

All differences greater than 1 σ are high, except for PNL-3

Is PST-9 (case 3a) a valid data point or an outlier?

Unreflected Spheres of Plutonium-Nitrate Solutions



⇒ Thermal cross sections for ^{239}Pu should be reviewed

REFLECTED HEU NITRATE SOLUTION WITH Cd

Source	k_{eff}	Δk
Benchmark	1.0012 ± 0.0019	—
ENDF/B-VI	0.9870 ± 0.0004	-0.0142 ± 0.0016
ENDF/B-VII.0	0.9918 ± 0.0004	-0.0094 ± 0.0016
ENDF/B-VII.0 + NNDC ^{113}Cd	1.0008 ± 0.0004	-0.0004 ± 0.0016

$|\Delta k| > 5\ \sigma$

Benchmark is a reflected HEU nitrate solution in water that has a thermal spectrum even though cadmium is present in the solution

Reactivity deficiency was traced to problems with the ^{113}Cd cross sections, and a new evaluation for ^{113}Cd was generated by the National Nuclear Data Center at Brookhaven National Laboratory

CONCLUSIONS

Improvements still are needed, particularly for:

- ^{235}U cross sections in the unresolved resonance region
- Fast copper cross section
- Neptunium cross sections
- Angular scattering distribution for ^{2}H (probably)
- Thermal plutonium (^{239}Pu) cross sections

One problem already has been resolved:

- Thermal ^{113}Cd cross sections

New cross sections for ^{113}Cd will be included in the next interim distribution, ENDF/B-VII.1

LA-UR-07-2053

MCNPX 2.6.X Features (2006-2007)

by

Gregg McKinney, Joe Durkee, John Hendricks, Mike James, Russ Johns, Denise Pelowitz, and Laurie Waters

M&C/SNA 2007, Monterey, CA, April 15-19, 2007

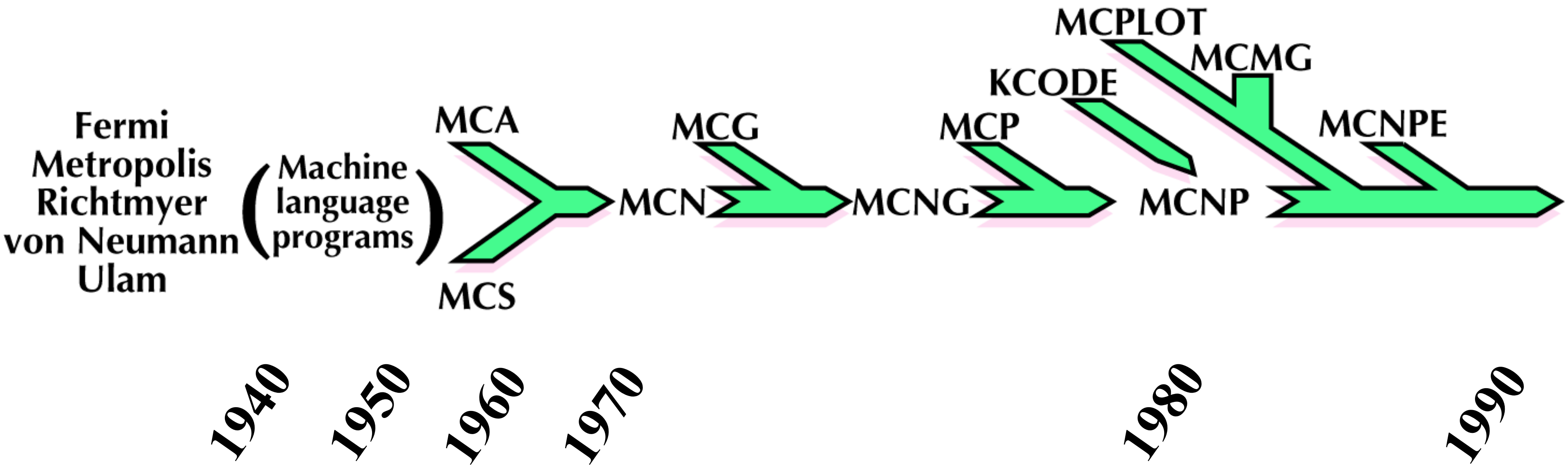
MCNPX 2.6.X Features (2006-2007)

- MCNPX Overview
- History of MCNPX
- User Base
- Features for 2006-2007
- Future of MCNPX

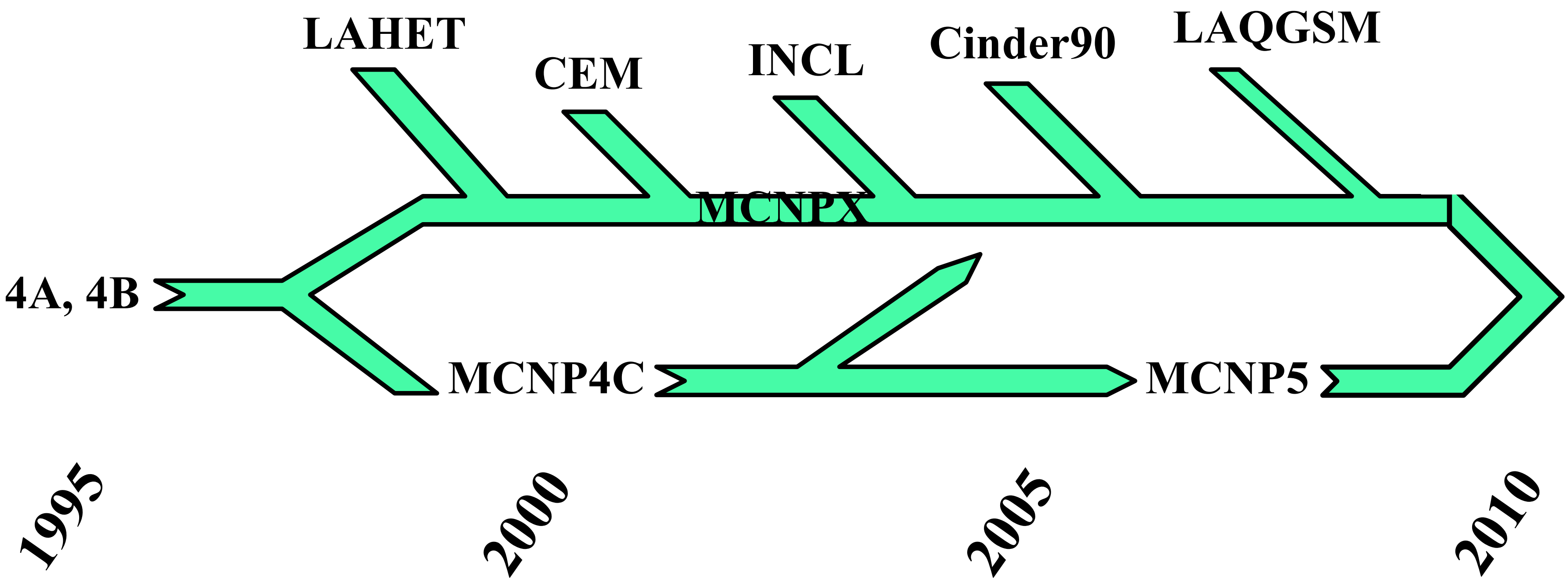
MCNPX Overview

- 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
  - 1^{st} & 2^{nd} 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 transmutation

Version 2.6.C December, 2006

Spherical weight windows, delayed particle production

Version 2.6.D ~May, 2007

Coupled space-energy-time WW, radioactive sources, LAQGSM

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

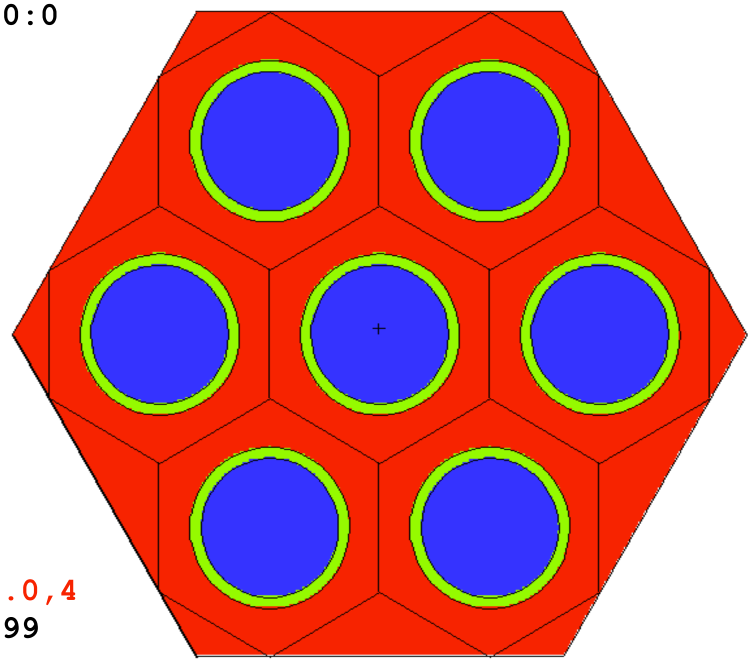
Application	# Groups	Percent
Medical (BNCT, proton therapy, etc.)	**50**	**15**
Spacecraft, Cosmic Rays, SEE, propulsion	**42**	**12**
Detectors, experiments, Threat Reduction	**39**	**11**
ATW, ADS, Energy Amplifiers	**37**	**11**
Fuel cycles, beginning to end, including storage	**32**	**9**
Accelerator 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**

Features for 2006 – Version 2.6.A

- Transmutation using Cinder90 (BURN card)
  - Several keywords of options (MAT, POWER, etc.)
  - Automatic updating of material atom densities
- 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
2   8   -6.5     1 -2       u=1 imp:n=1
3   9   -0.7       2        u=1 imp:n=1
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 1.3 0 150 -1.3 0 150 0.66 1.14 150
      0.66 -1.14 150 -0.66 1.14 150 -0.66 -1.14 150
```



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

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
```

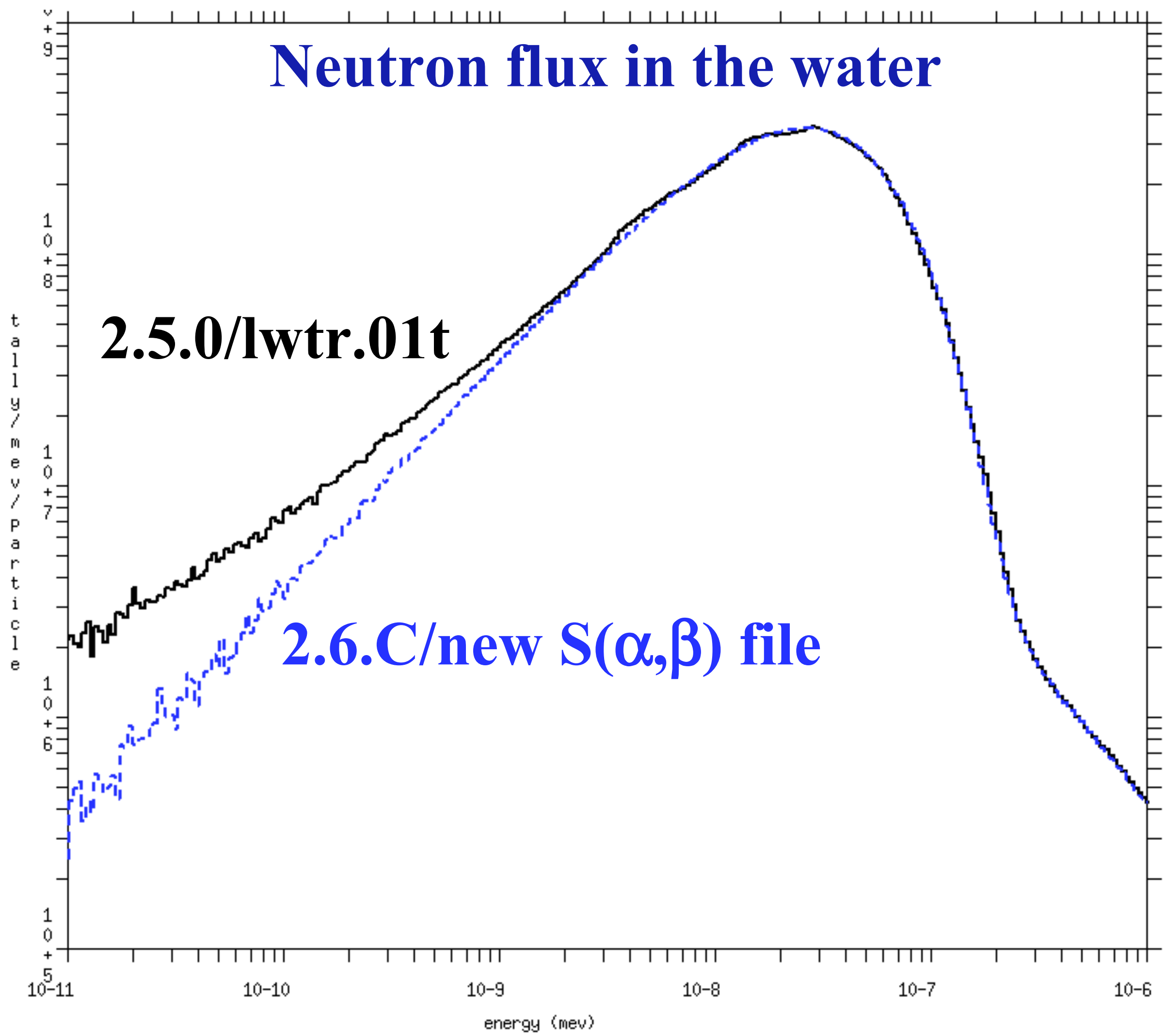
OUTPUT FILE

```
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  $ Replace with lwtr.01t for old 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

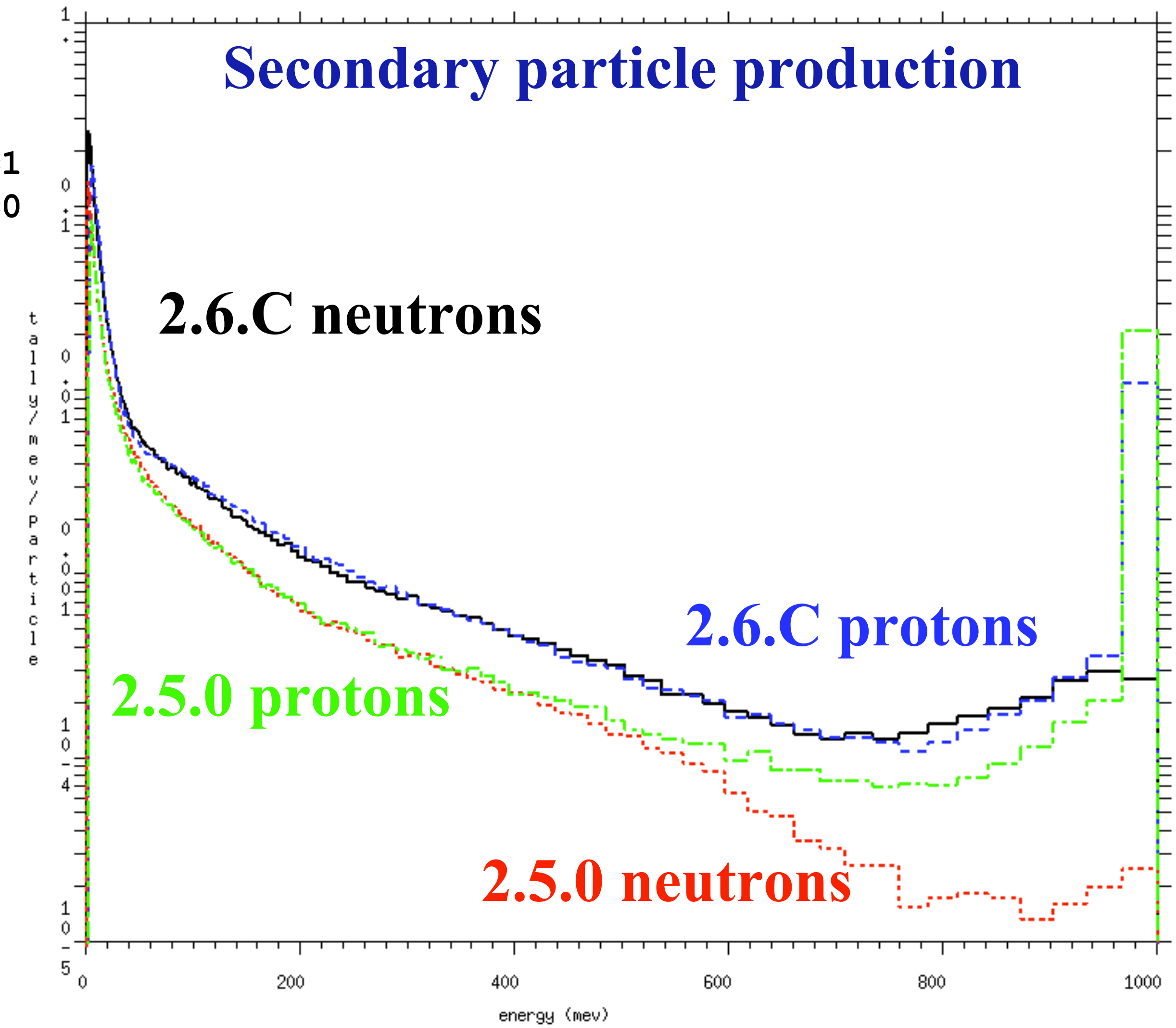


Features for 2006 – Version 2.6.B

- Transmutation improvements (BURN card)
  - 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

CEM Upgrade

```
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
```



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.

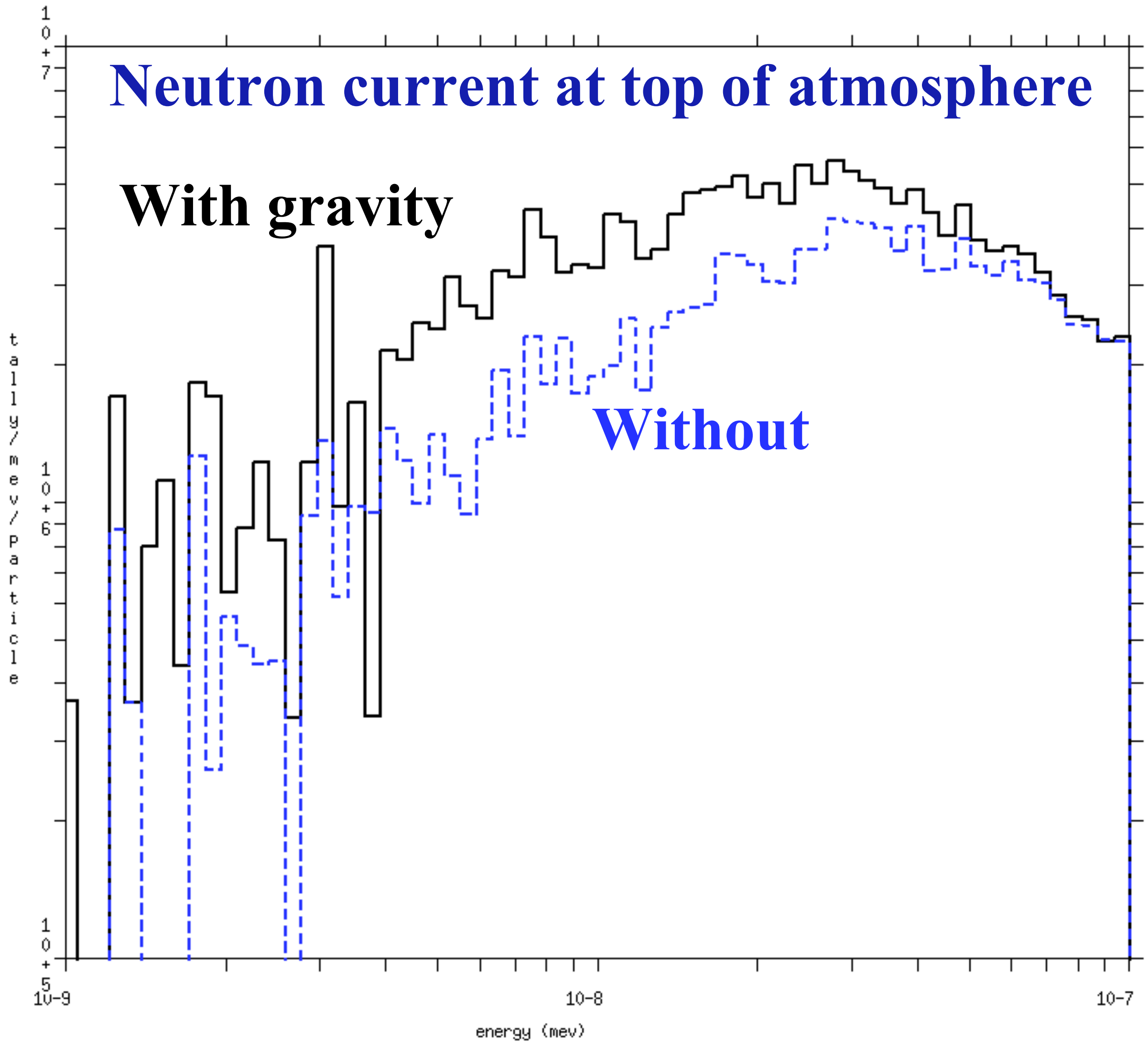
FIELD Card

```
5 GeV protons into Mars, 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
```

```
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



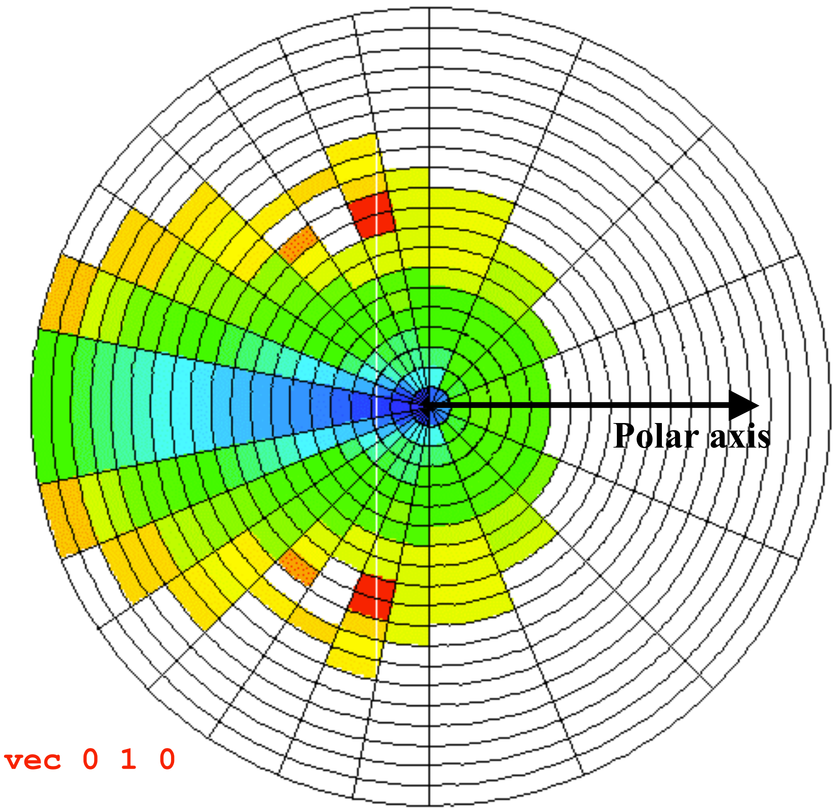
Neutron current at top of atmosphere
With gravity
Without
tally/mev/particle
10+7
10+6
10+5
10-9
10-8
10-7
energy (mev)

Features for 2006 – Version 2.6.C

- Transmutation improvements (BURN card)
  - Support for continue-runs & parallel execution
  - 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

Spherical Weight Windows

```
10 MeV photons into 1m H2O surrounding 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
```



Delayed Neutrons and Gammas

```
DN/DG from high-energy fission of U-235
1 1 -18.9 -1     imp:n=1
2 0        +1     imp:n=0

1 sph  0 0 0 0.1

mode n p
m1    92235.60c -1
phys:n 20 2j 101 20
phys:p 5j -102
cut:n  j j 0 0
sdef  erg=10.0 par=n
f01:p 1
e01   .100 499i 12.
t01   0.0001e8 100.e8
f11:p 1
t11   0.0000001e8 99log 100.e8
f21:n 1
e21   .001 199log 12.
t21   0.0001e8 100.e8
f31:n 1
t31   0.0000001e8 99log 100.e8
nps   2000000
```

Delayed Neutrons and Gammas

neutron creation	tracks	weight (per source particle)	energy (per source particle)
source	2000000	1.0000E+00	1.0000E+01
nucl. interaction	0	0.	0.
particle decay	0	0.	0.
weight window	0	0.	0.
cell importance	0	0.	0.
weight cutoff	0	0.	0.
energy importance	0	0.	0.
dxtran	0	0.	0.
forced collisions	0	0.	0.
exp. transform	0	0.	0.
upscattering	0	0.	0.
photonuclear	0	0.	0.
(n,xn)	22458	1.1229E-02	1.2686E-02
prompt fission	65553	3.2679E-02	6.7772E-02
delayed fission	15331	1.2414E-04	5.7533E-05
tabular boundary	0	0.	0.
tabular sampling	0	0.	0.
total	2103342	1.0440E+00	1.0081E+01

neutron loss	tracks	weight (per source particle)	energy (per source particle)
escape	2078492	1.0317E+00	9.9508E+00
energy cutoff	0	0.	0.
time cutoff	0	0.	0.
weight window	0	0.	0.
cell importance	0	0.	0.
weight cutoff	0	0.	0.
energy importance	0	0.	0.
dxtran	0	0.	0.
forced collisions	0	0.	0.
exp. transform	0	0.	0.
downscattering	0	0.	8.1324E-03
capture	98	3.8100E-05	1.6678E-04
loss to (n,xn)	7486	3.7430E-03	3.7421E-02
loss to fission	17266	8.5948E-03	8.4020E-02
nucl. interaction	0	0.	0.
particle decay	0	0.	0.
tabular boundary	0	0.	0.
total	2103342	1.0440E+00	1.0081E+01

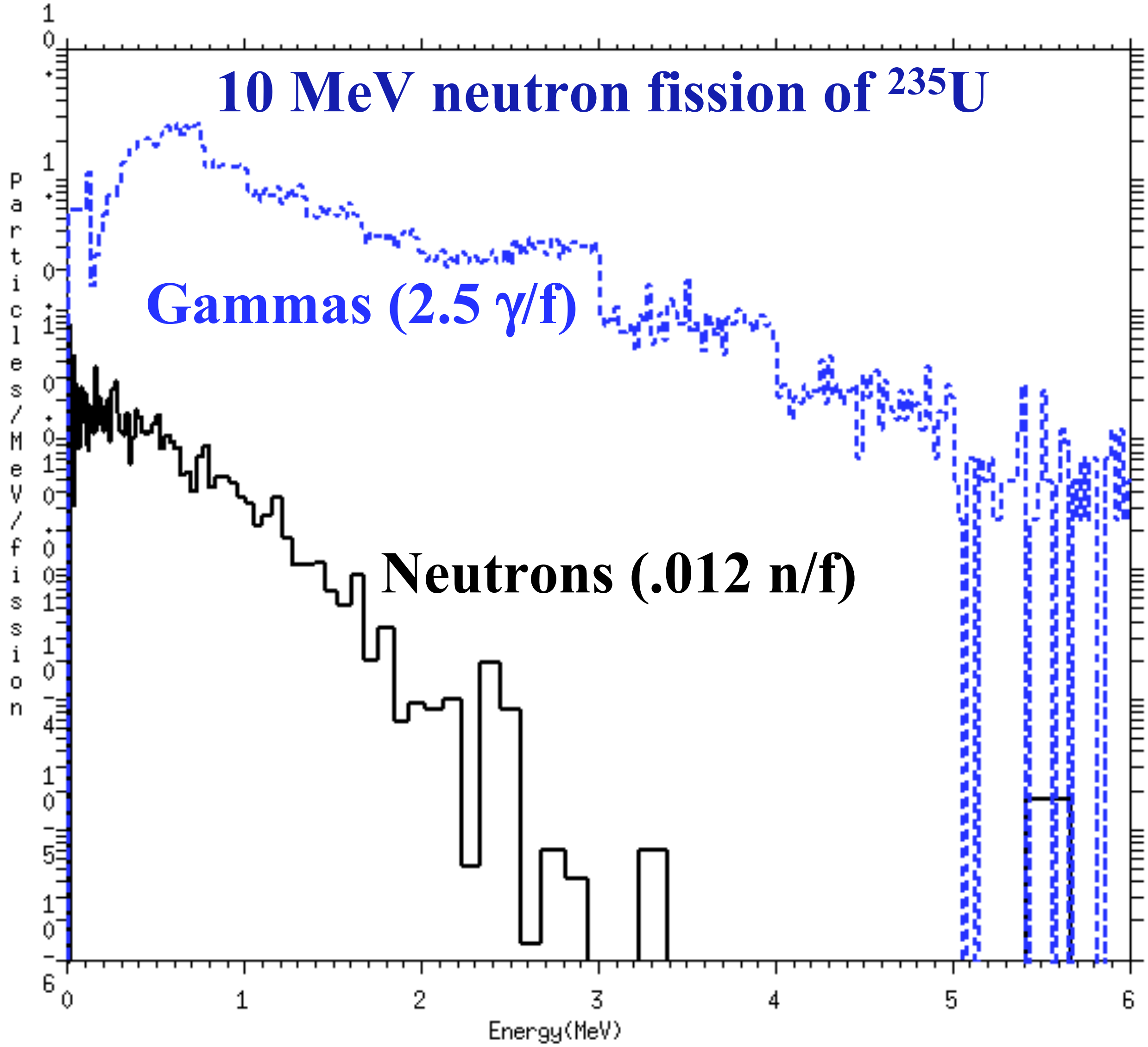
photon creation	tracks	weight (per source particle)	energy (per source particle)
source	0	0.	0.
nucl. interaction	0	0.	0.
particle decay	113751	5.6552E-02	5.4380E-02
weight window	0	0.	0.

photon loss	tracks	weight (per source particle)	energy (per source particle)
escape	127772	1.2601E-01	1.3541E-01
energy cutoff	1	2.0234E-06	5.2097E-06
time cutoff	0	0.	0.
weight window	0	0.	0.

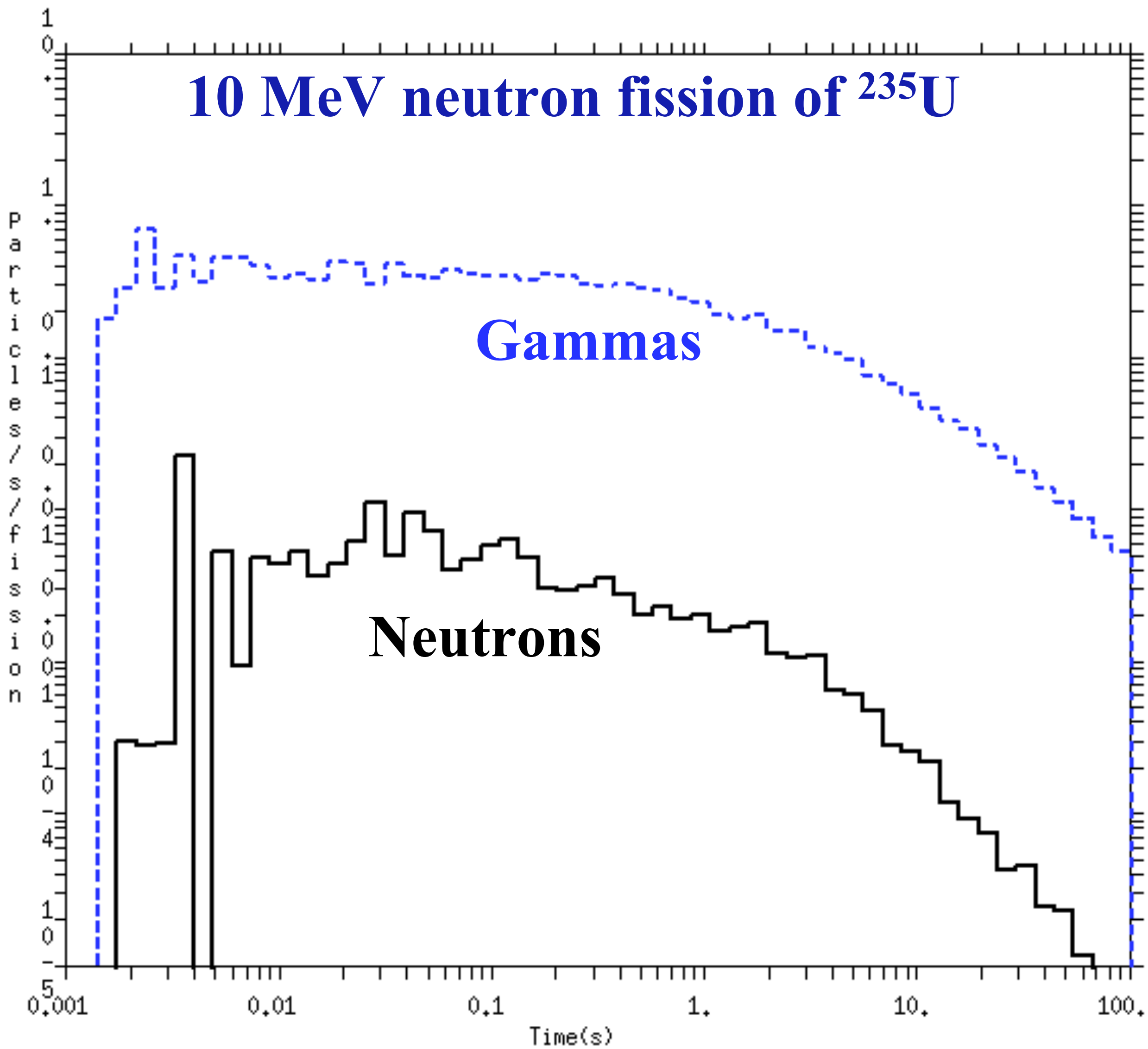
Total DG = 6.6 γ/f

Total DN = .014 n/f

Delayed Neutrons and Gammas

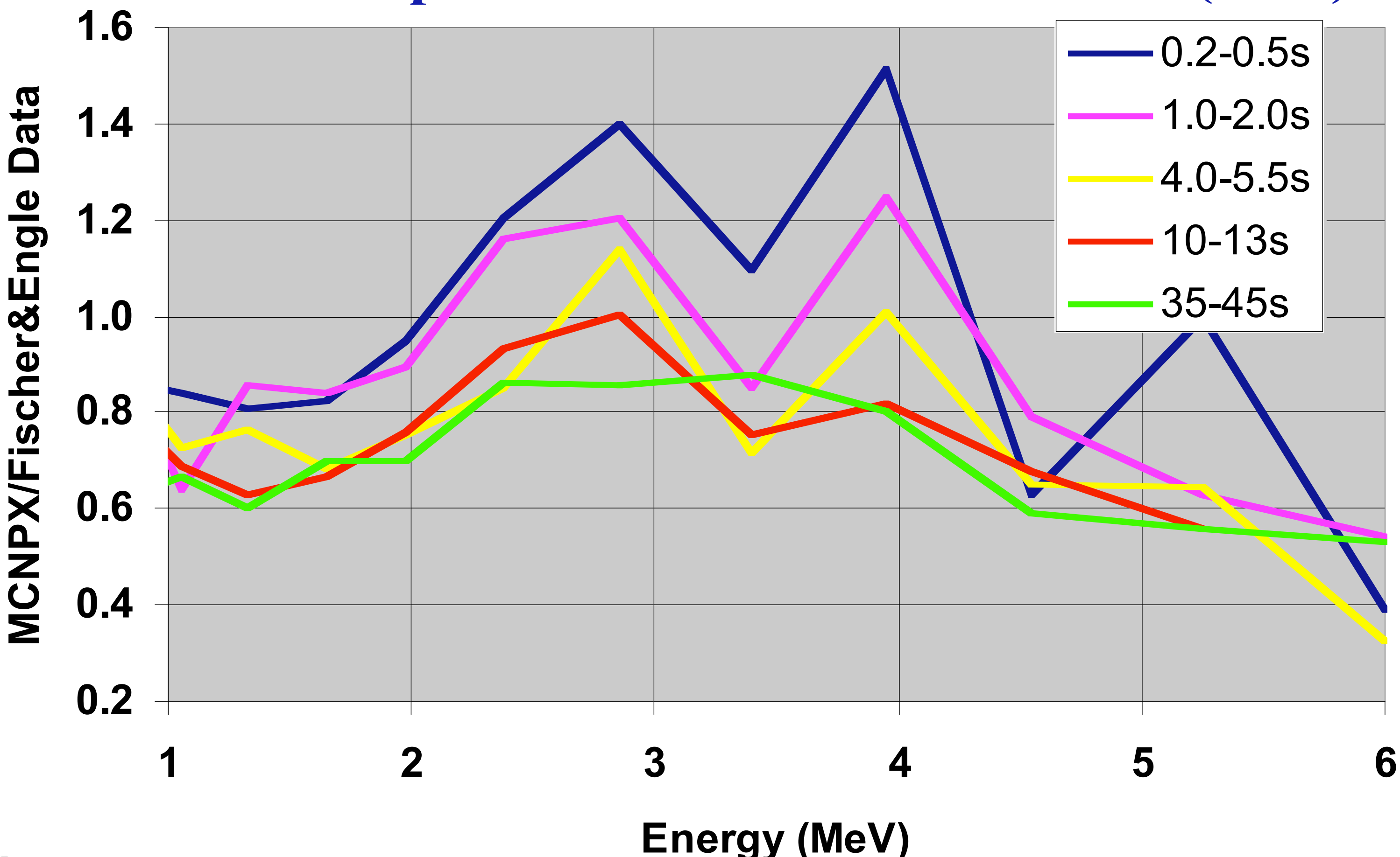


Delayed Neutrons and Gammas



Delayed Neutrons and Gammas

C/E comparison to measured ^{235}U data (1964)



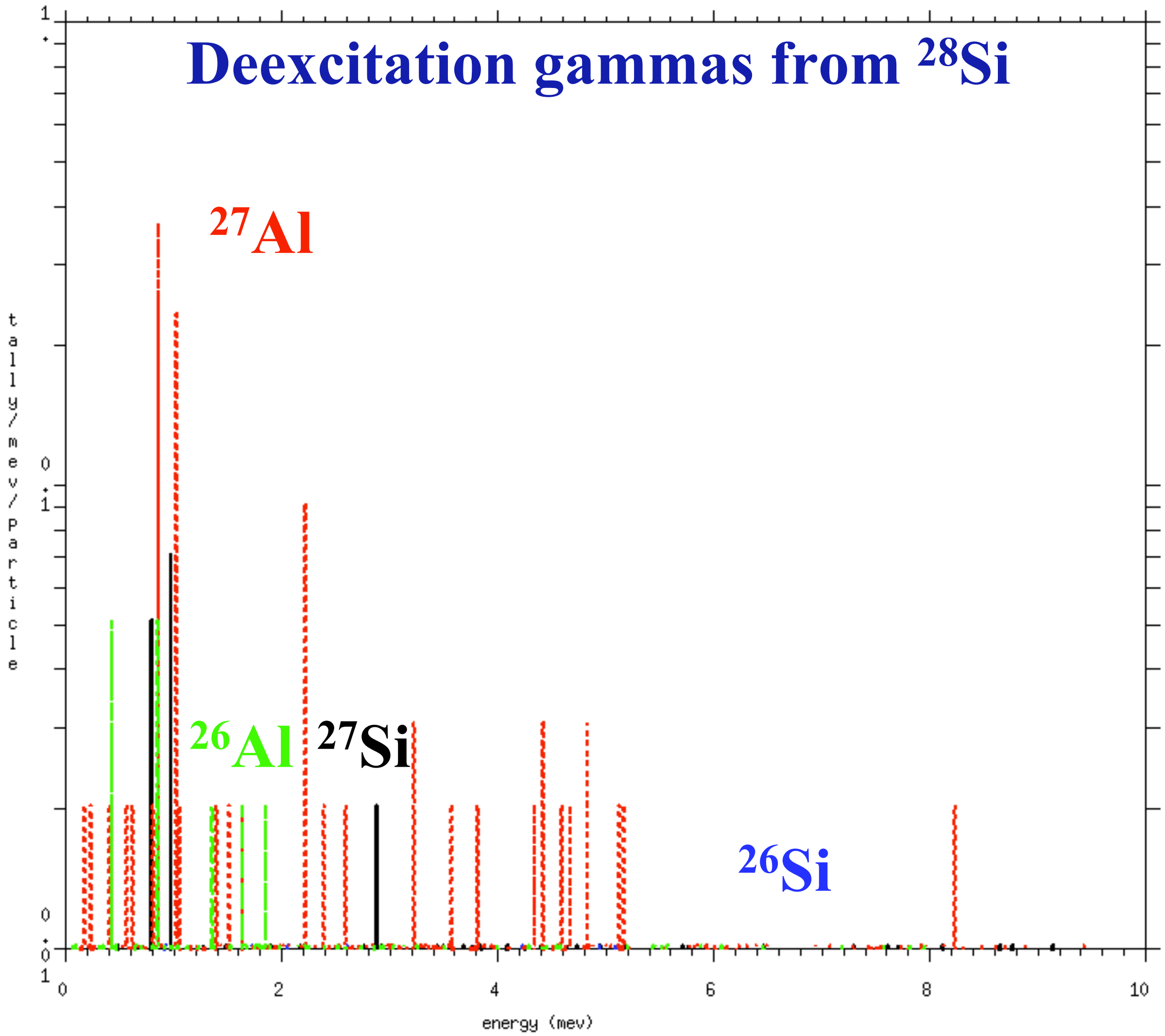
Photon Tally Tagging

```
5 GeV protons into Mars 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
```

```
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

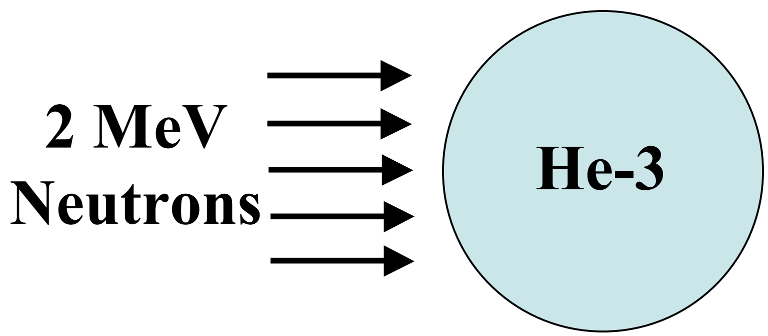
Photon Tally Tagging



Models for Library Interactions

```
2 MeV neutrons into He-3
1  1 -5.3540E-4  -1     imp:n=1
2  0              1 -2  imp:n=1
3  0              2     imp:n=0

1  so 4.0
2  so 100.0

mode   n h d t s
sdef   par=n erg=2 pos=-5 0 0 rad=d1
       axs=1 0 0 ext=0 vec=1 0 0 dir=1
si1    0 3
sp1    -21 1
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
```

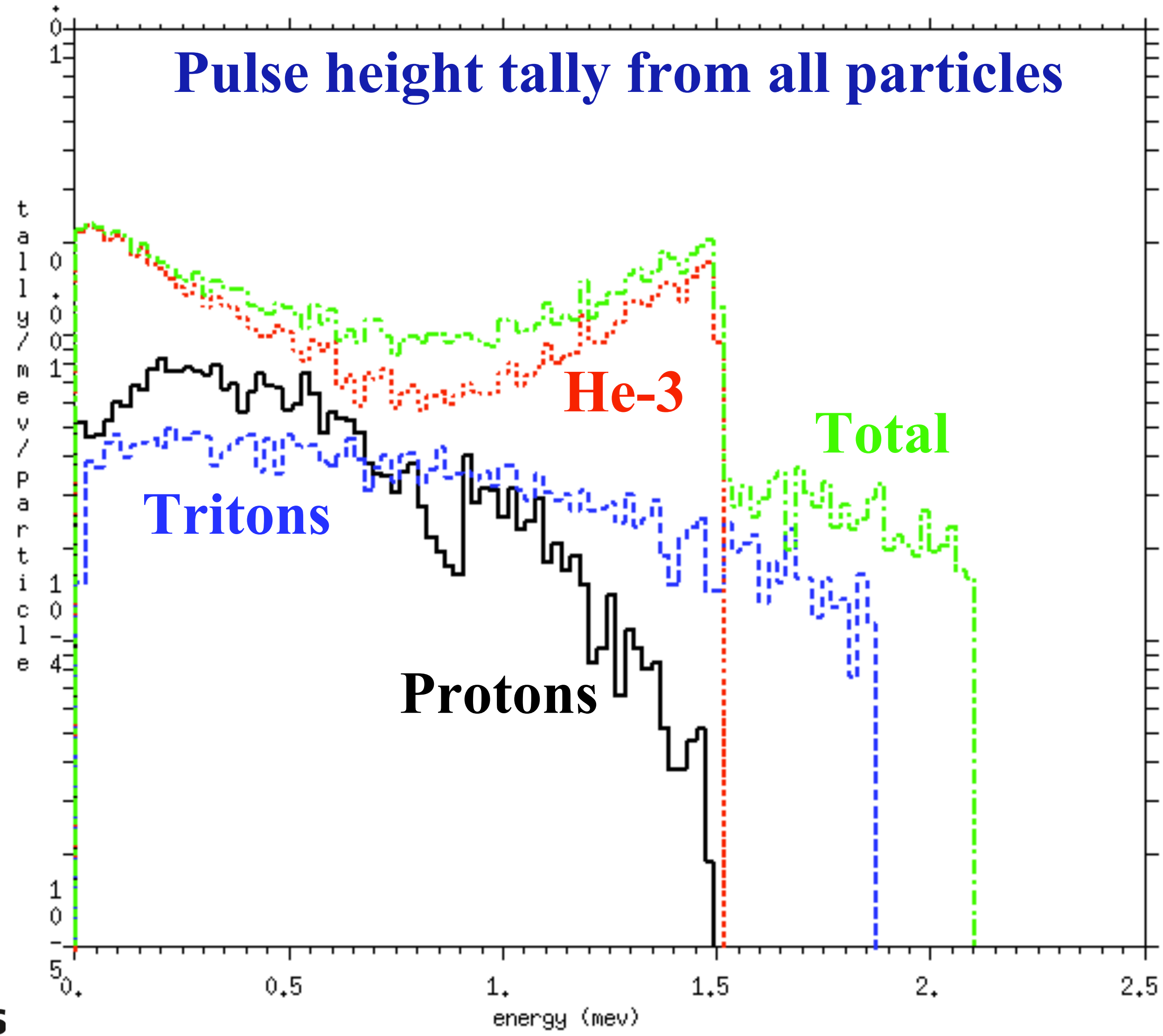
```
f8:n   1
e8     0. 99i 2.1
ft8    PHL 1  6 1 0
f18:n 1
e18    0. 99i 2.1
ft18   PHL 1 16 1 0
f28:n 1
e28    0. 99i 2.1
ft28   PHL 1 26 1 0
f38:n 1
e38    0. 99i 2.1
ft38   PHL 1 36 1 0
f58:n 1
e58    0. 99i 2.1
ft58   PHL 4 6 1 16 1 26 1 36 1 0
```



LA150N Library

Isotope	ZAID	Proton	Deuteron	Triton	Alpha
H-1	1001.24c	1.0E-11			
H-2	1002.24c	3.339		1.0E-11	
Be-9	4009.24c	14.266	16.301	11.709	0.667
C	6000.24c	20.0	20.0		20.0
N-14	7014.24c	20.0	20.00		20.0
O-16	8016.24c	20.0	20.0		20.0
Al-27	13027.24c	1.897	6.274	11.29	3.25
Si-28	14028.24c	4.0	20.0	20.0	2.746
Si-29	14029.24c	3.0	20.0	20.0	1.3
Si-30	14030.24c	8.012	20.0	20.0	4.345
P-31	15031.24c	20.0	20.0		20.0
Ca	20000.24c	20.0	20.0	20.0	20.0
Cr-50	24050.24c	1.0	20.0	20.0	2.25
Cr-52	24052.24c	3.256	20.0	20.0	1.233
Cr-53	24053.24c	2.69	20.0	20.0	1.0
Cr-54	24054.24c	6.33	20.0	20.0	1.581
Fe-54	26054.24c	0.7	20.0	20.0	3.0
Fe-56	26056.24c	2.966	20.0	20.0	0.862
Fe-57	26057.24c	1.943	20.0	20.0	0.8
Ni-58	28058.24c	0.5	20.0	20.0	0.5

Models for Library Interactions



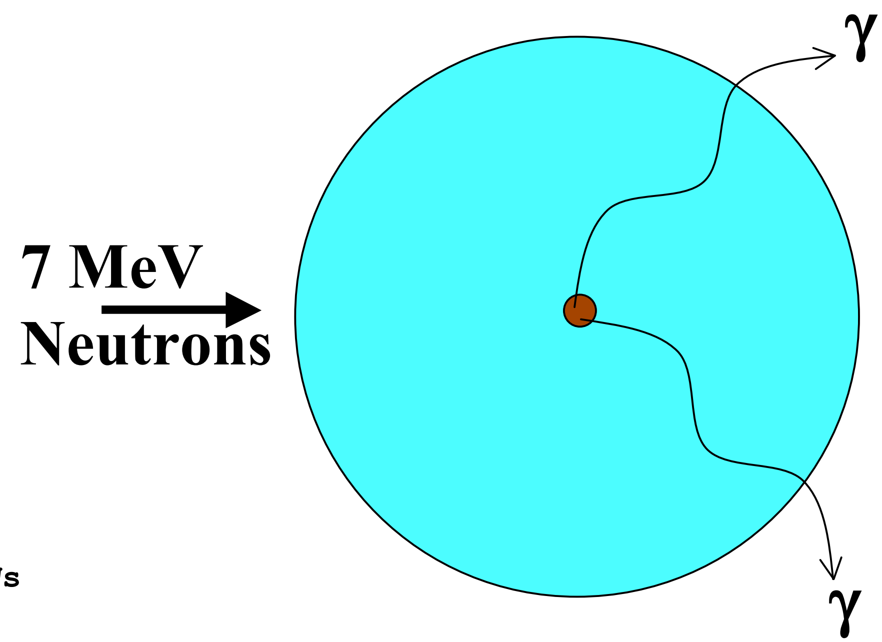
UNCLASSIFIED

Features for 2007 – Version 2.6.D

- Transmutation improvements (BURN card)
  - Time-dependent material changes (CONC keyword)
  - Repeated-structures power norm. (VOL keyword)
  - Fission-product tier improvements
- Coupled space-energy-time weight windows
- Activation neutrons and gammas
- Background radioactive sources
- Muon capture physics
- Heavy-ion transport (via LAQGSM)

Coupled Space-Energy-Time WW

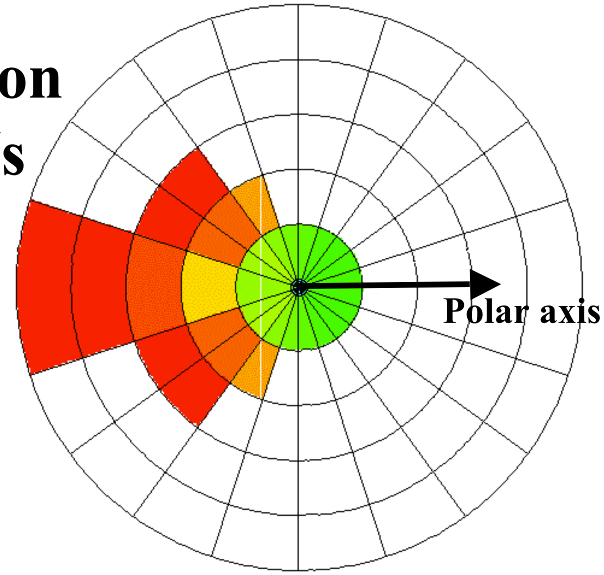
```
7 MeV neutrons into H2O surrounding 2kg HEU
1   1   -19.0    -1     imp:n=1
2   2   -1.0     +1 -2  imp:n=1
3   0               +2  imp:n=0

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

mode n p
phys:p 5j -101  $ turn on delayed gammas
sdef par=n erg=7 pos=-99 1 1 vec=1 0 0 dir=1
m1    92235 .5 92238 .5
m2    1001 2 8016 1
nps 100000
f1:p 2
t1    0.1e8 1e15 nt
f4:n 1
wwg 4 0
mesh geom=rpt origin=0 0 0 ref=-99 1 1
     axs=1 0 0 vec=0 1 0
     imesh  3.01 101.  iints  3 5
     jmesh   .5 jints  10
     kmesh   1  kints  1
c    wwp:n  4j -1 $ Add this to use neutron WWs
```



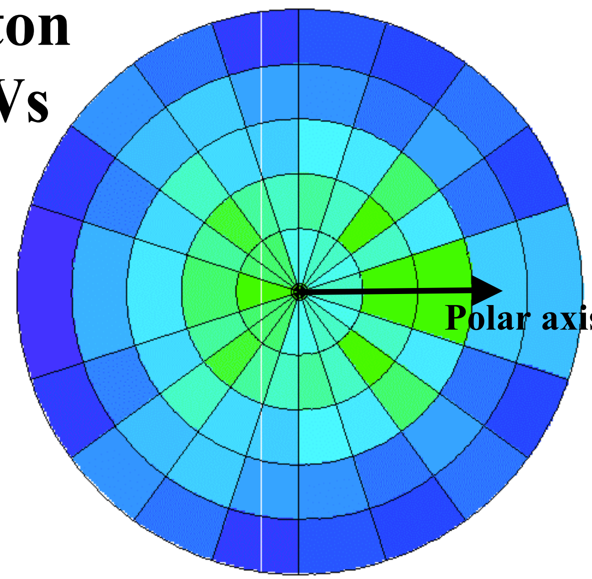
Coupled Space-Energy-Time WW

```
7 MeV neutrons into H2O surrounding 2kg HEU
1  1  -19.0   -1    imp:n,p=1
2  2  -1.0    +1 -2 imp:n,p=1
3  0             +2 imp:n,p=0

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

mode n p
totnu no
phys:p j 1 3j -101  $ turn on delayed gammas
sdef par=n erg=7 pos=-99 1 1 vec=1 0 0 dir=1
m1   92235 .5 92238 .5
m2   1001 2 8016 1
nps  300000
f1:p 2
t1   0.1e8 1e15 nt
e1   3 100 nt
wwg  1 0 5j 1
wwge:p 0.1e8 1e15
mesh geom=rpt origin=0 0 0 ref=-99 1 1 axs=1 0 0 vec=0 1 0
     imesh  3.01 101.  iints  3 5
     jmesh   .5 jints  10
     kmesh   1  kints  1
wwp:n 4j -1
c    wwp:p  4j -1 $ Add this to use photon WWs
```

Neutron WWs

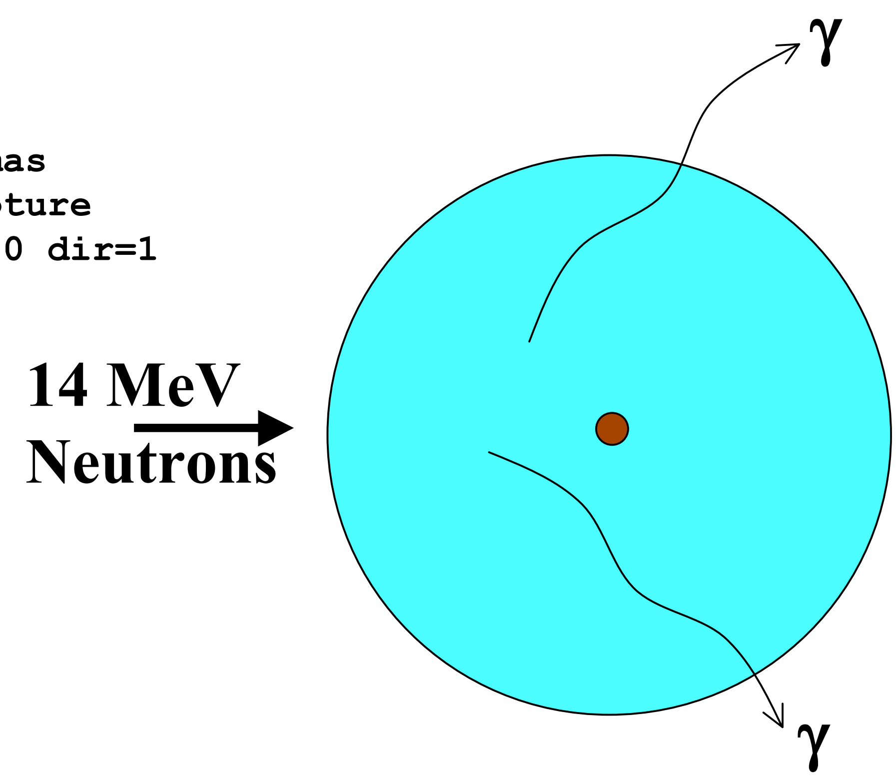


Photon WWs

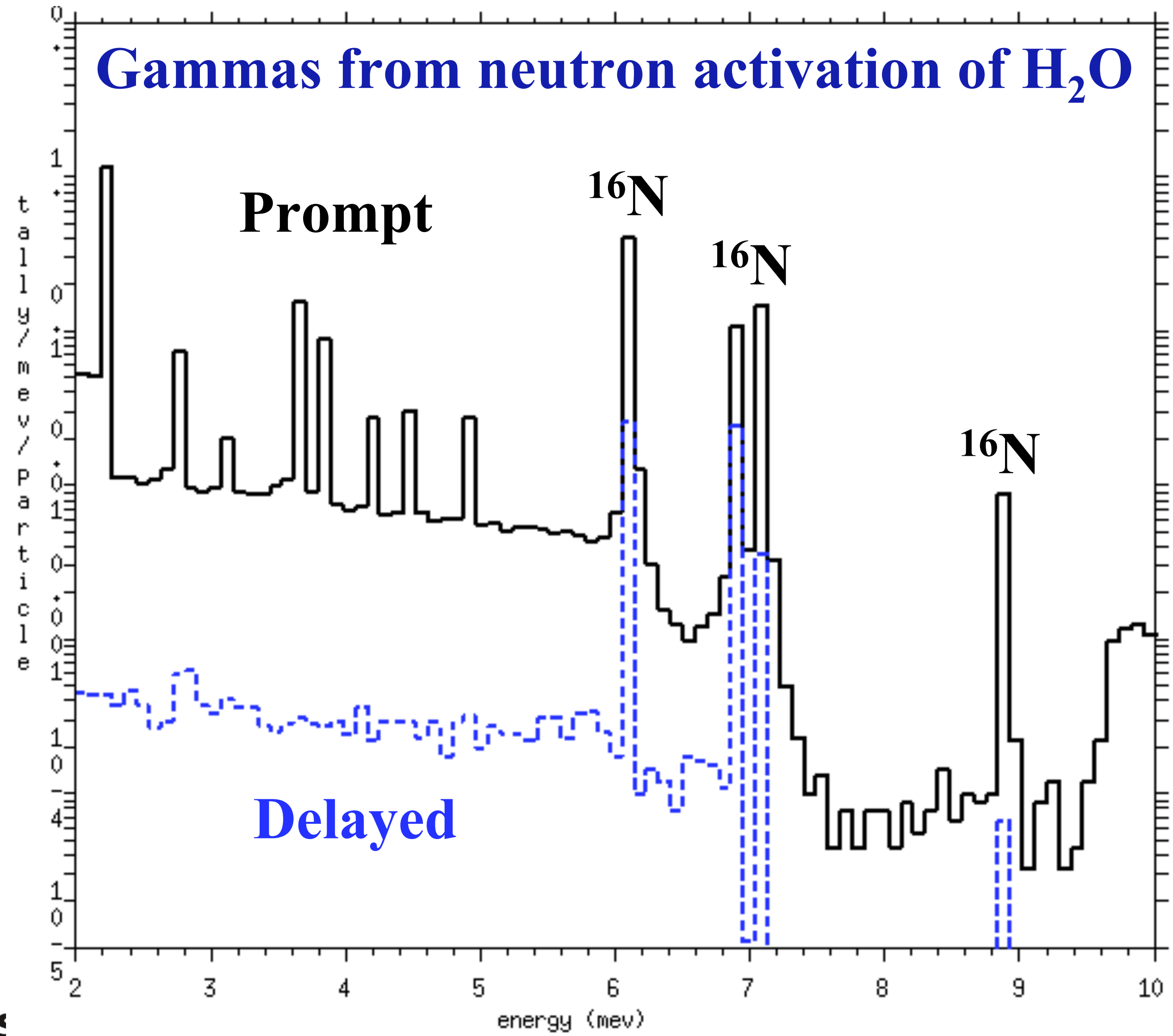


Activation Neutrons & Gammas

```
14 MeV neutrons into H2O surrounding 2kg HEU
1  1  -19.0   -1     imp:n,p=0
2  2  -1.0    +1 -2  imp:n,p=1
3  0             +2  imp:n,p=0

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

mode n p
phys:p 5j -102  $ turn on delayed gammas
cut:n  2j 0 0  $ turn off implicit capture
sdef par=n erg=14 pos=-99 1 1 vec=1 0 0 dir=1
m1   92235 .5 92238 .5
m2   1001 2 8016 1
nps 1000000
f1:p 2
t1   0.1e8 1e15 nt
e1   1 99i 10
```



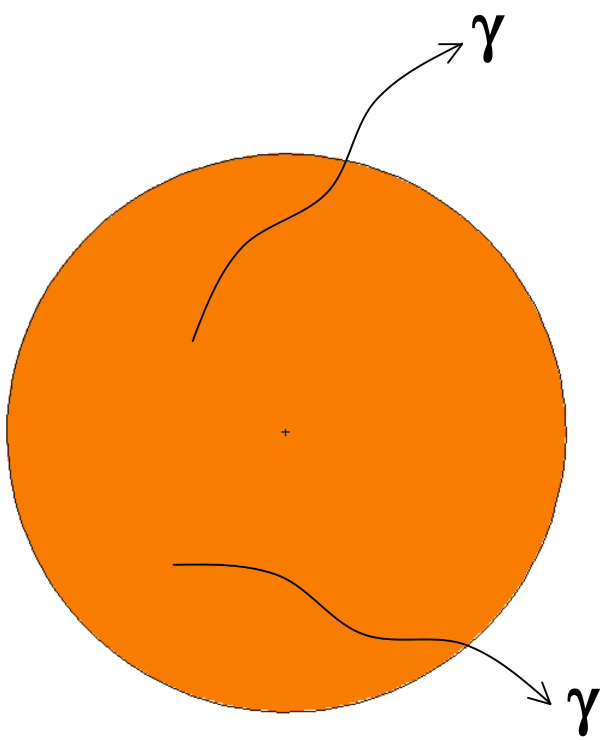
Activation Neutrons & Gammas



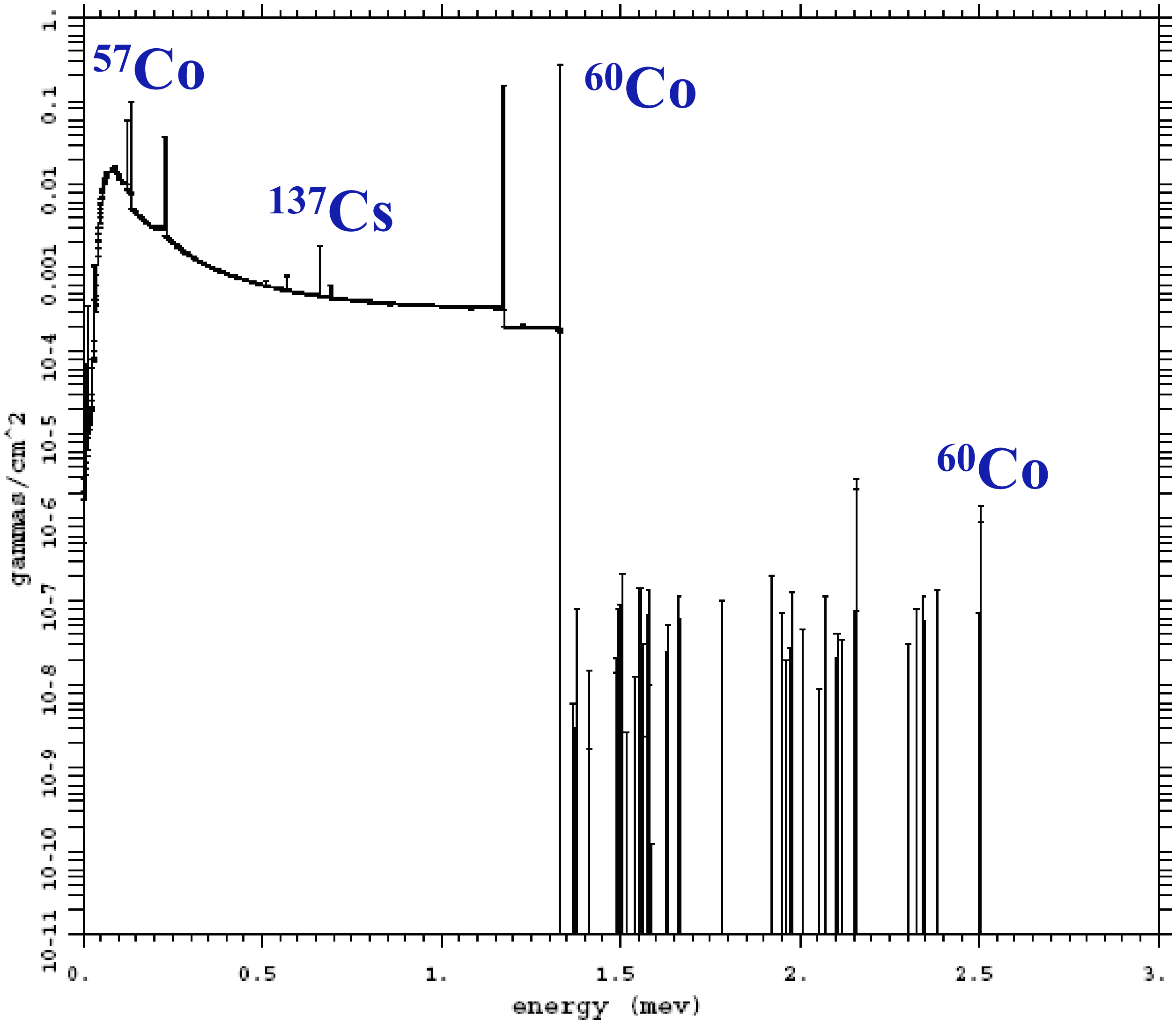
UNCLASSIFIED

Background Radioactive Sources

```
Co-57, Co-60, and Cs-137 within soil
1 2 -1.6  -1      imp:p=1
2 0        1      imp:p=0

1 so 100.0

sdef par=sp cel=1 pos=0 0 0 wgt=1 rad=d1
si1 0 100
sp1 -21 2
mode p
nps 100000
m2    1001.66c  -.002  8016.66c -.527
      11023.66c -.021 13027.66c -.061
      14028     -.345 19000     -.029
      26056 -.016
      27057 -0.00000001 27060 -.000001
      55137 -.000323
      plib=.02p
e0 0.0 2999i 3.0
f4:p 1
f2:p 1
c2 0 1
```



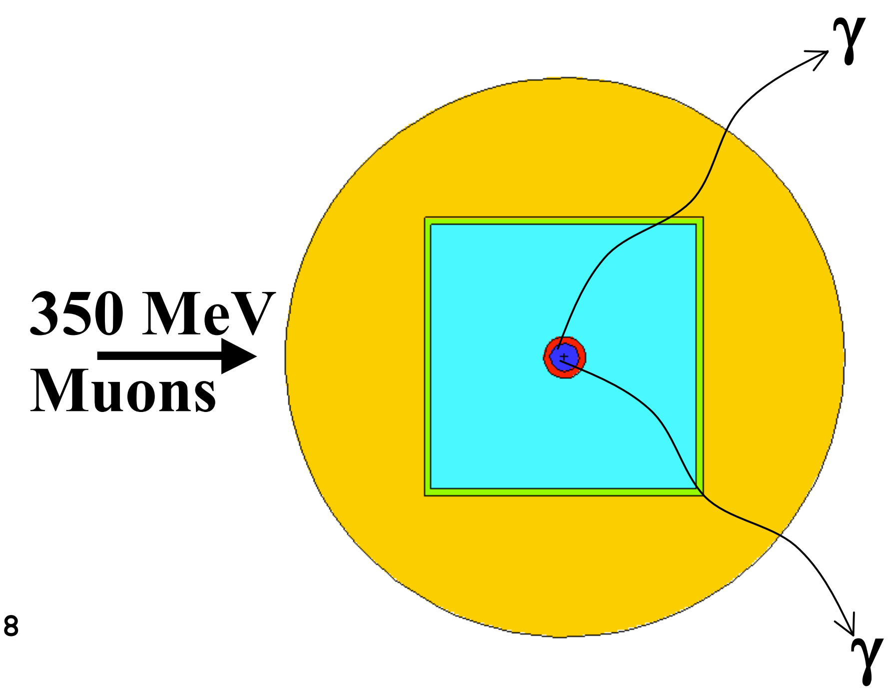
Background Radioactive Sources



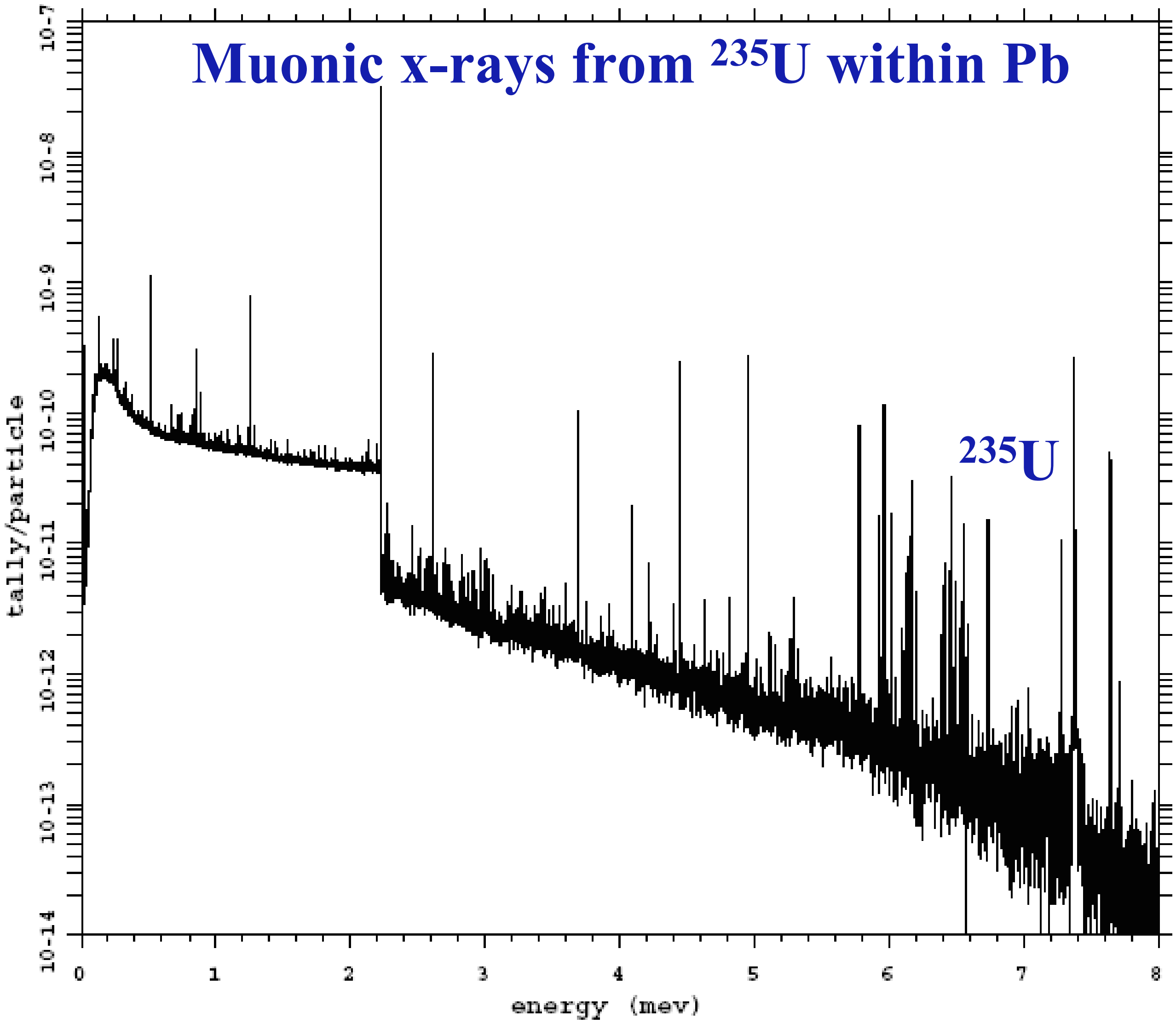
Muon Capture Physics

```
350 MeV muons into Pb surrounding HEU
1 1 -18.95   -1          imp:|,p=1
2 8 -11.35   1 -2        imp:|,p=1
3 3 -1.0   2 -3          imp:|,p=1
4 4 -7.8 3 -4            imp:|,p=1
5 5 -1.205e-3   4 -100   imp:|,p=1
100 0  100               imp:|,p=0

1 rcc -10.0 0.0 0.0 20.0 0.0 0.0 5.0
2 rcc -12.5 0.0 0.0 25.0 0.0 0.0 7.5
3 rpp -47.5 47.5 -47.5 47.5 -47.5 47.5
4 rpp -50.0 50.0 -50.0 50.0 -50.0 50.0
100 so   100.0

mode |  p
phys:| 350.0
phys:p 350.0
sdef par=| erg=350.0 x=d1 y=d2 z=-60.0
     vec=0 0 1 dir=1
si1 -12.5 12.5
sp1 0  1
si2 -7.5 7.5
sp2 0  1
m1  92238 -.20 92235 -.80
m3  1001 2     6012 1
m4  26054 5.9 26056 91.72 26057 2.1 26058 .28
```

```
m5    1000 -6e-4 8000 -0.2353 7000 -0.7513
     18000 -0.0128
m8   82204 1.4   82206 24.1    82207 22.1
     82208 52.4
e2 0.0 9999i 10.0
f2:p 100
```



Muon Capture Physics

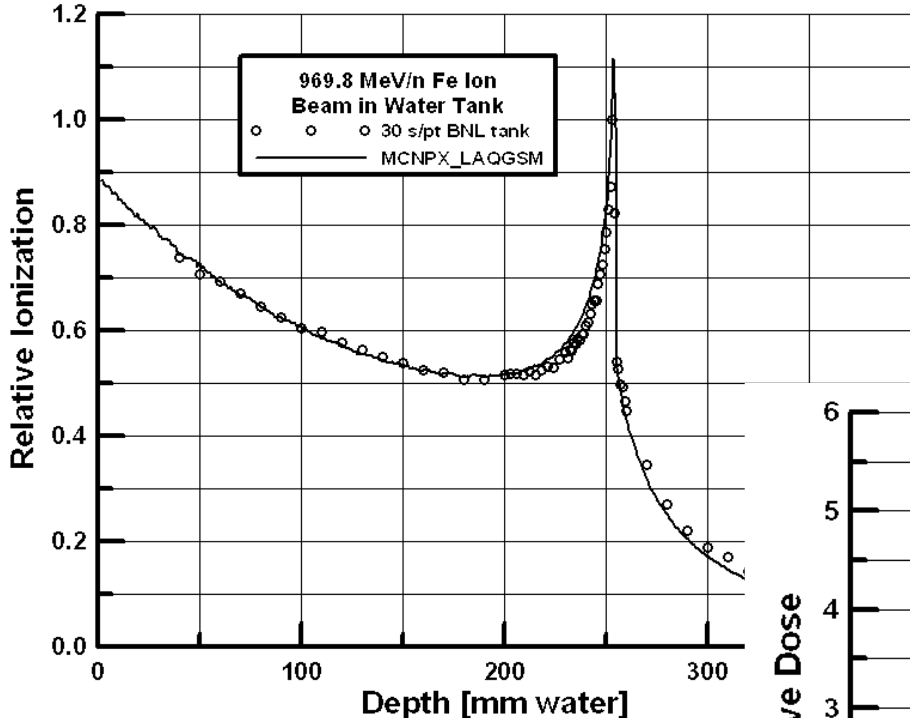


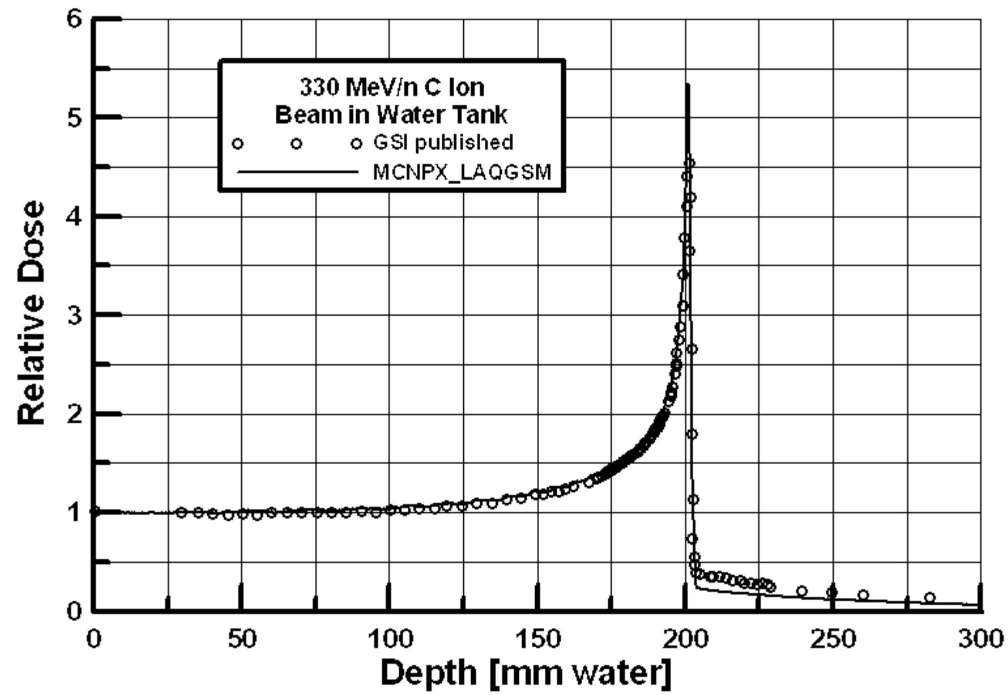
Heavy-ion Transport

```
969 MeV/n Fe into H2O
1       2  -1.0      -1      imp:n=1
2       1  -0.0012    1   -2 imp:n=1
3       0                  2 imp:n=0

1       rpp -15 15 -15 15 0 40.0
2       rcc 0 0 -20   0 0 80 50
3       pz -1

m1      7014.24h 0.781 8016.24h 0.219
m2      1001.24h 0.667 8016.24h 0.333
mode    h a n #
phys:h 60000 j j j j j 0.1
phys:n 60000 j 0 -1 j j 1
lca 8j 3
sdef    par=26056 erg=d2 sur=3 dir=1 vec=0 0 1 pos=0 0 -1 rad=d1
si1     0 0.5
sp1     -21
si2     L 54224.00 54251.00 54278.00
sp2     0.25 0.5 0.25
nps     20000
tmesh
rmesh3 total
cora3  -7.0   7.0
corb3  -7.0   7.0
corc3   0.0  400i   40.0
endmd
```

Undocumented Feature?

Heavy-ion Transport





Features for 2007 – Version 2.6.E

- Transmutation improvements
  - Accurate evolution of meta-stables
  - Treatment for minor actinides
- Plotting of spherical mesh tallies
- Enhanced tally tagging (other particles & tags)
- Time-dependent transformations
  - Allows moving universes (e.g., control-rod movement)
- Fission gamma multiplicity
- Nuclear resonance fluorescence physics

Future of MCNPX

- Possible public release of 2.6.0 (~Sept. 2007)
- MCNPX and MCNP merger
  - Hope to preserve all features of both codes
  - Preliminary version by Summer 2007
  - Public release perhaps in 2008
- Capabilities beyond 2.6.0 will be put in MCNP6/7
  - MCNPX will cease to be distributed
  - MCNP web site may allow for a small Beta group
  - MCNP & MCNPX workshops will be combined