

MCNP/X Transport in the Tabular Regime

H. Grady Hughes

Los Alamos National Laboratory

Hadronic Shower Simulation Workshop

Fermilab, 6-8 September 2006

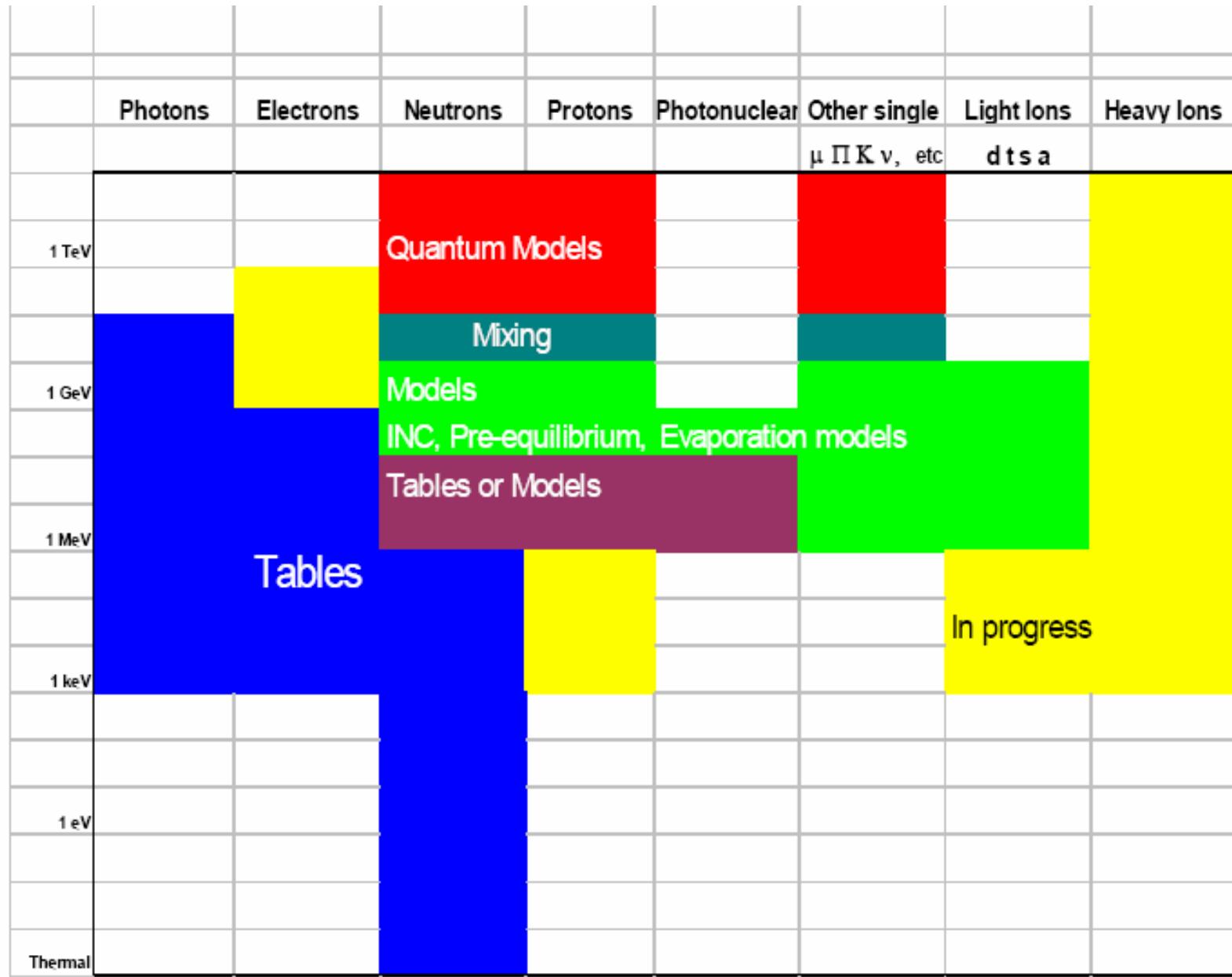
Abstract

In this presentation, I shall review the transport capabilities of the MCNP and MCNPX Monte Carlo codes in the energy regimes in which tabular transport data are available. Giving special attention to neutron tables, I shall emphasize the measures taken to improve the treatment of a variety of difficult aspects of the transport problem, including unresolved resonances, thermal issues, and the availability of suitable cross section sets. I shall also briefly touch on the current situation in regard to photon, electron, and proton transport tables, and mention anticipated data libraries expected in the near future.

What are the tabular regimes?

- Neutrons: 10^{-11} MeV – 150MeV
- Photons (photo-atomic): 1 keV – 100 GeV
- Photons (photo-nuclear): threshold – 150 MeV
- Electrons: 1 keV – 1 GeV
- Protons: 1 MeV – 150 MeV

MCNP/X Tables and Models



Why are low energies of interest?

- Low-energy experimental background
- Facility shielding design
- Beam dump design
- Calorimeter — complete description
- Spallation sources
- Isotope production/destruction
- Air and groundwater activation
- etc.

Transport tables are well-suited for . . .

- Energy-deposition calculations
- Dosimetry
- Shielding design
- Predicting radiation backgrounds
- Radiography simulations
- Detector calibration
- Criticality safety
- Reactor design
- Predicting material damage

Transport tables are not well-suited for . . .

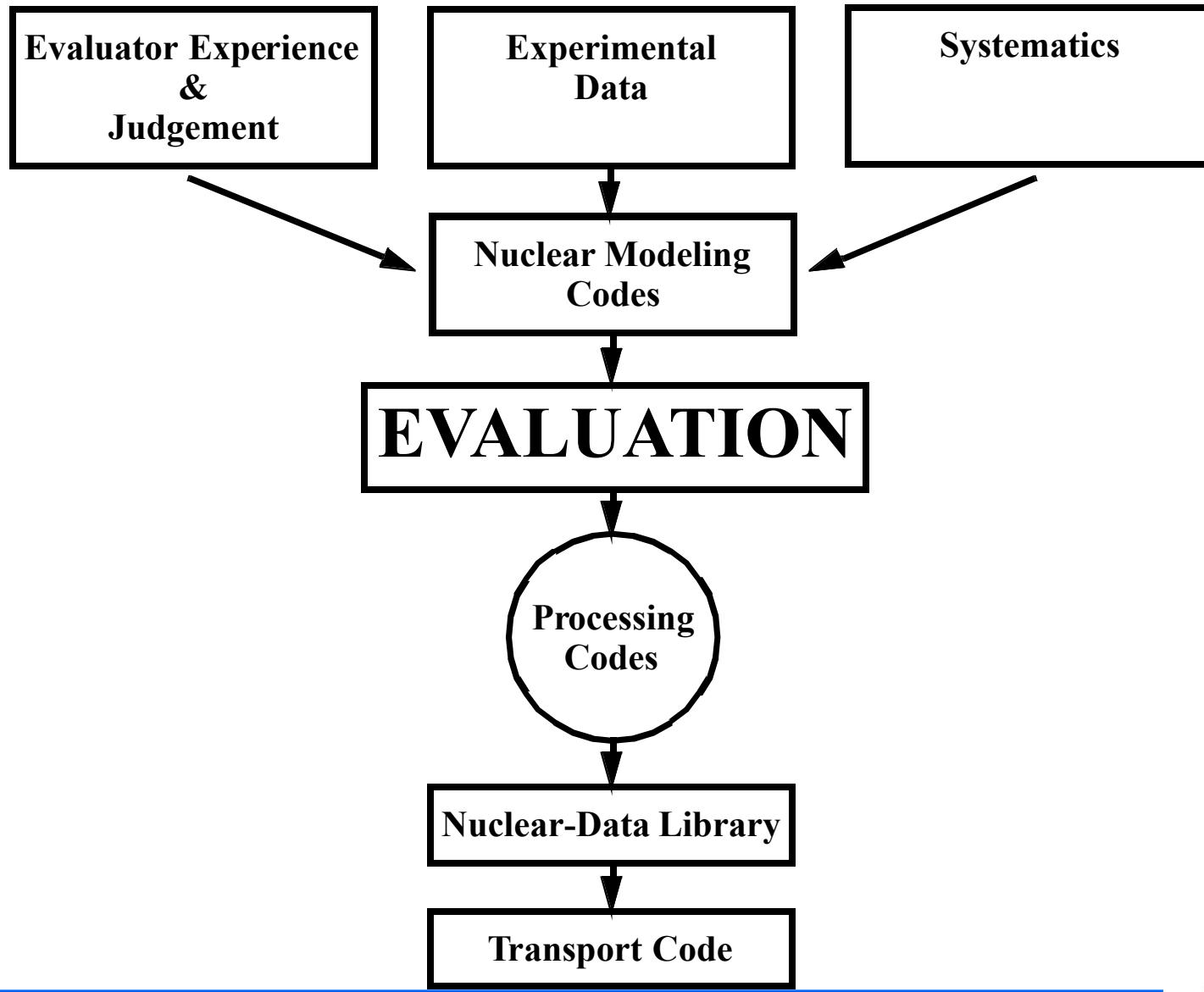
Simulation of coincidence experiments

(at least ENDF-based tables)

There are many kinds of tables

- Continuous-energy cross sections
- Multigroup cross sections
- Photonuclear cross sections
- Thermal transport tables
- Neutron dosimetry tables
- Decay chain data
- Other physical data

Where do cross sections come from?



Nuclear Data Evaluations – Compilations

- ENDF/B (Evaluated Nuclear Data File)
 - US National Effort
 - Currently Version VI
 - CSEWG
 - NNDC
- ENDL (Evaluated Nuclear Data Library - from LLNL)
- JEF (Joint European File)
- EFF (European File - Fusion)
- JEFF
- FENDL (Fusion ...)
- UK Nuclear Data Library
- JENDL (Japanese ...)
- CENDL (Chinese ...)
- BROND (Russian)
- Hansen-Roach Library

Necessary Cross-Section Data

For each particle being transported, cross sections are needed for:

- all target materials $\sigma=f(Z,A)$
- entire particle energy range $\sigma=f(Z,A,E_n)$
- each reaction, j $\sigma=f(Z,A,E_n,j)$

The above are sometimes referred to as “integrated” cross sections, which describe the probability of having an event. We also need differential cross sections to describe the outcome(s) of the event.

$$\sigma(Z;A;j;E_n, \Omega \rightarrow E', \Omega')$$

Nuclear Data Evaluations - Content

Complete, unambiguous description for particular combination of *incident particle* and *target* over a *specified energy range* (at least 10^{-11} MeV to 20 MeV for incident neutrons).

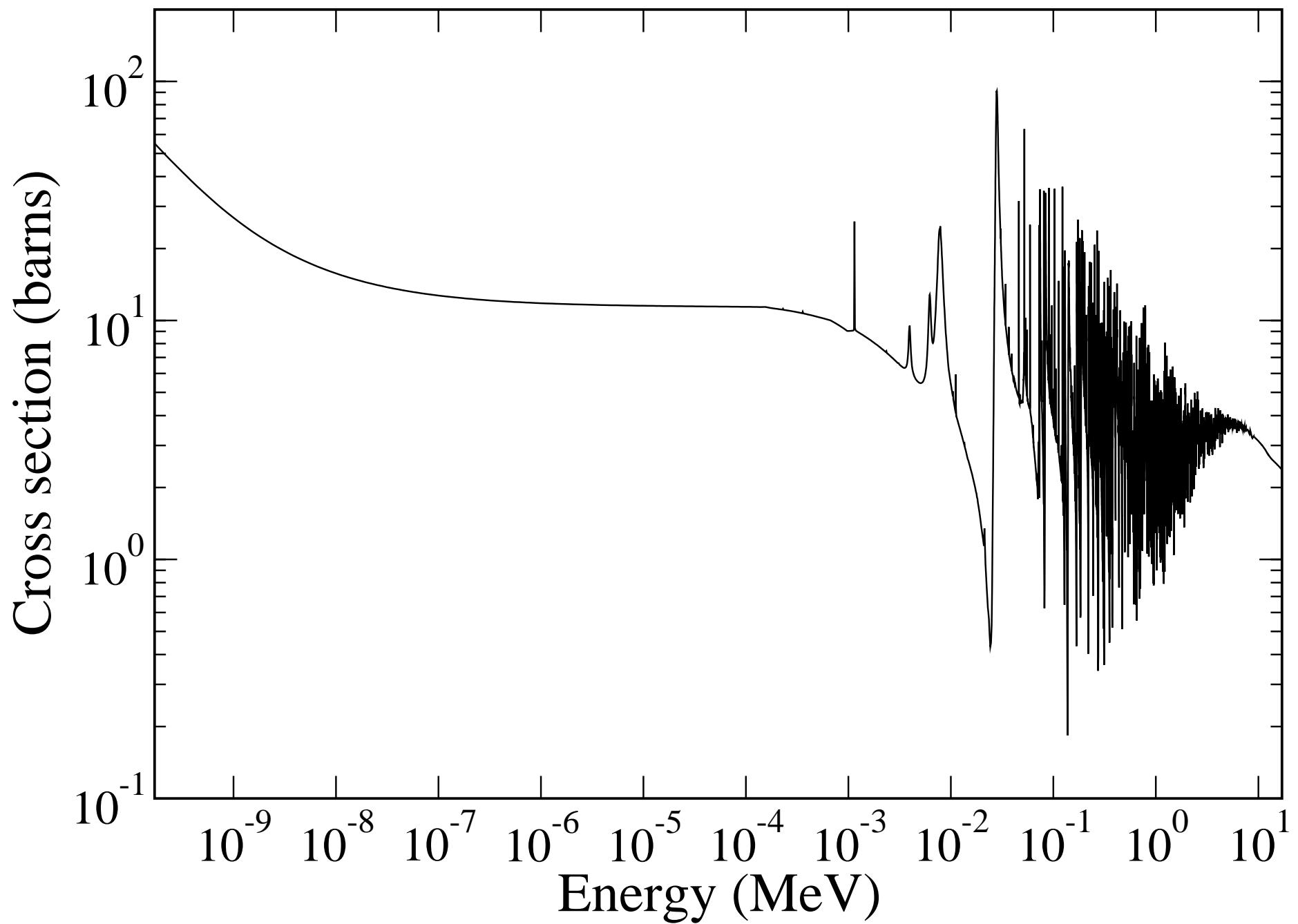
For each important reaction (all as a function of incident particle energy):

- integrated cross section
- multiplicity of each specified secondary particle
- angular and energy distributions for each specified secondary particle
- Q-value

Other Information:

- radioactive decay data
- fission-product yield data
- covariance data

Cross Section Example: Natural Iron Total XS From ENDF/B-V



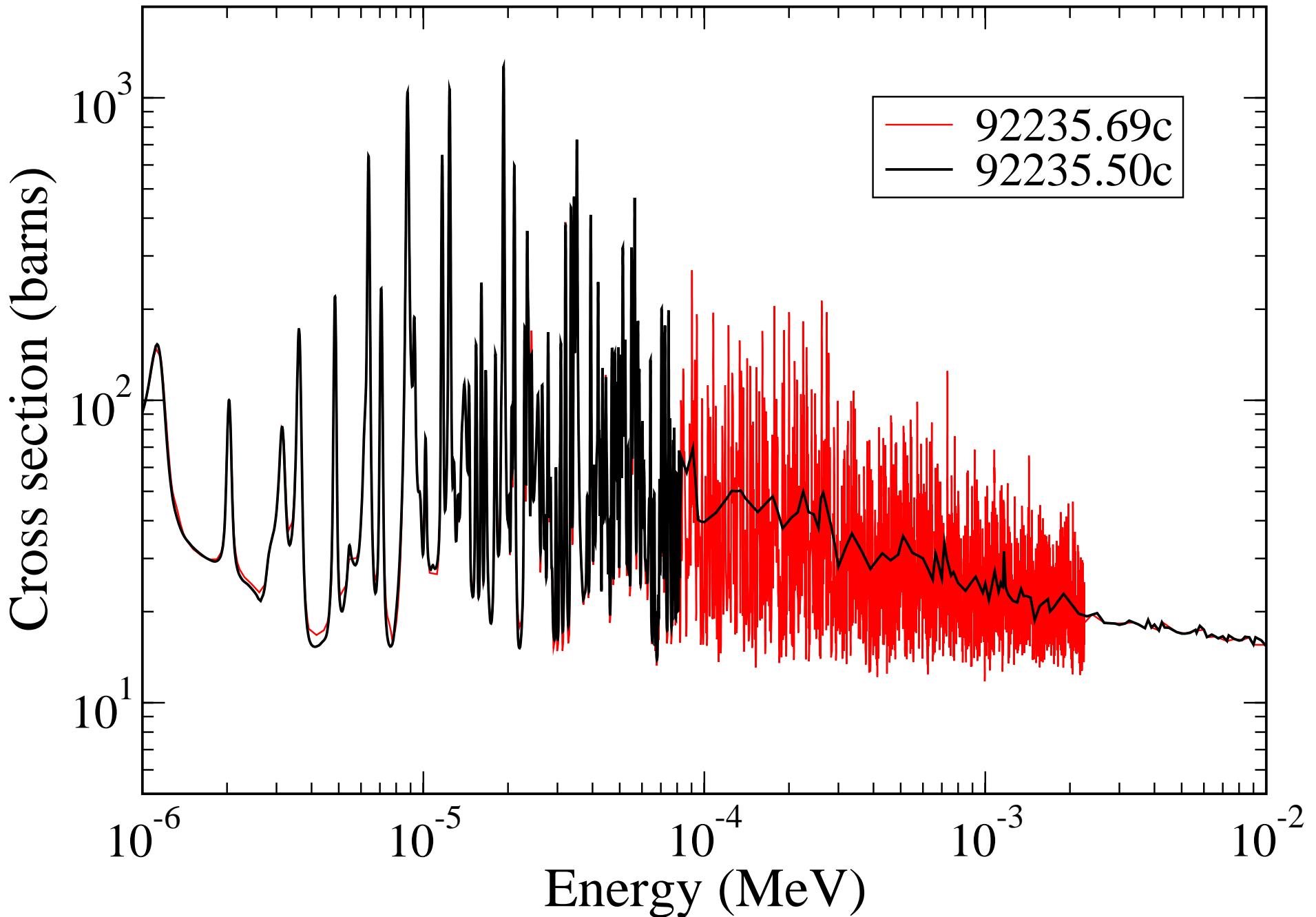
Some Neutron MT's (Reaction Identifiers)

<u>MT</u>	<u>EM</u>	<u>Description</u>
1	-1	Total
2	-3	Elastic
16		(n,2n)
17		(n,3n)
18	-6	Fission
51		(n,n') to 1st excited state
90		(n,n') to 40th excited state
91		(n,n') to continuum
101	-2	Total absorption (i.e., neutron disappearance)
102		Radiative capture (n, γ)
103		(n,p)
107		(n, α)
202	-5	Total photon production
301	-4	Average heating numbers (MeV/collision)

The unresolved resonance region

- For low- to medium- Z isotopes, the cross sections may be completely resolved in continuous-energy tables.
- For high- Z isotopes, the resonance region may be too complex to resolve with current data.
- Modern cross-section tables may provide probabilistic information for these regions.
- Recent versions of MCNP can make use of this probabilistic information.

ENDF/B-V and LANL T-16 U-235 Total Cross Section

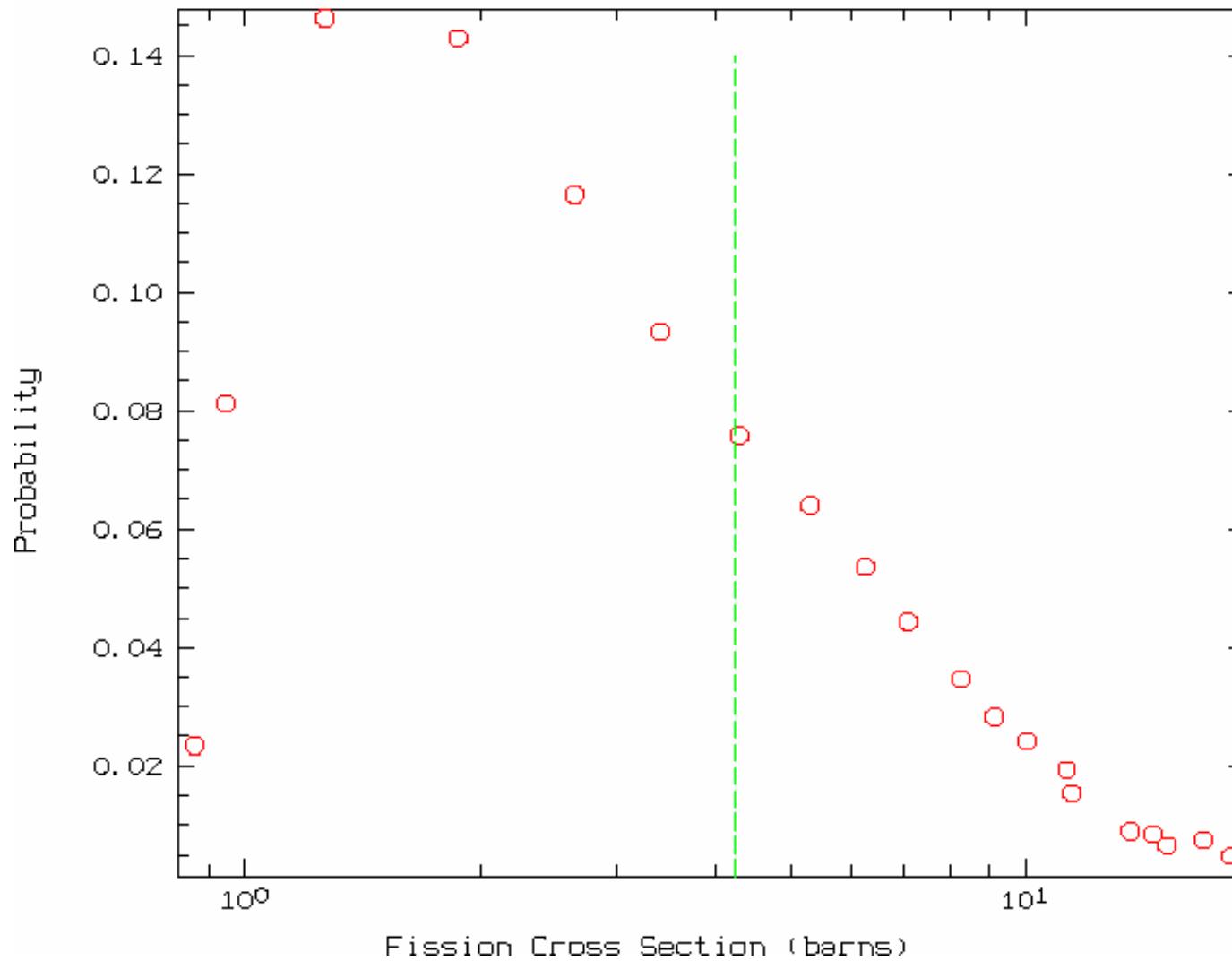


Unresolved Resonance Probability Tables

- MCNP4B and earlier
 - Average, infinitely-dilute cross sections were used in the unresolved energy range.
 - Therefore, any unresolved region self-shielding effects were not modeled correctly.
- MCNP4C, MCNPX, and later
 - Average cross sections are replaced by cross-section probability tables, which are derived from statistical information in evaluations such as average level spacings and average resonance widths.
 - When in the unresolved energy range, MCNP *samples* the cross sections from these probability tables.

Probability density in an unresolved resonance region

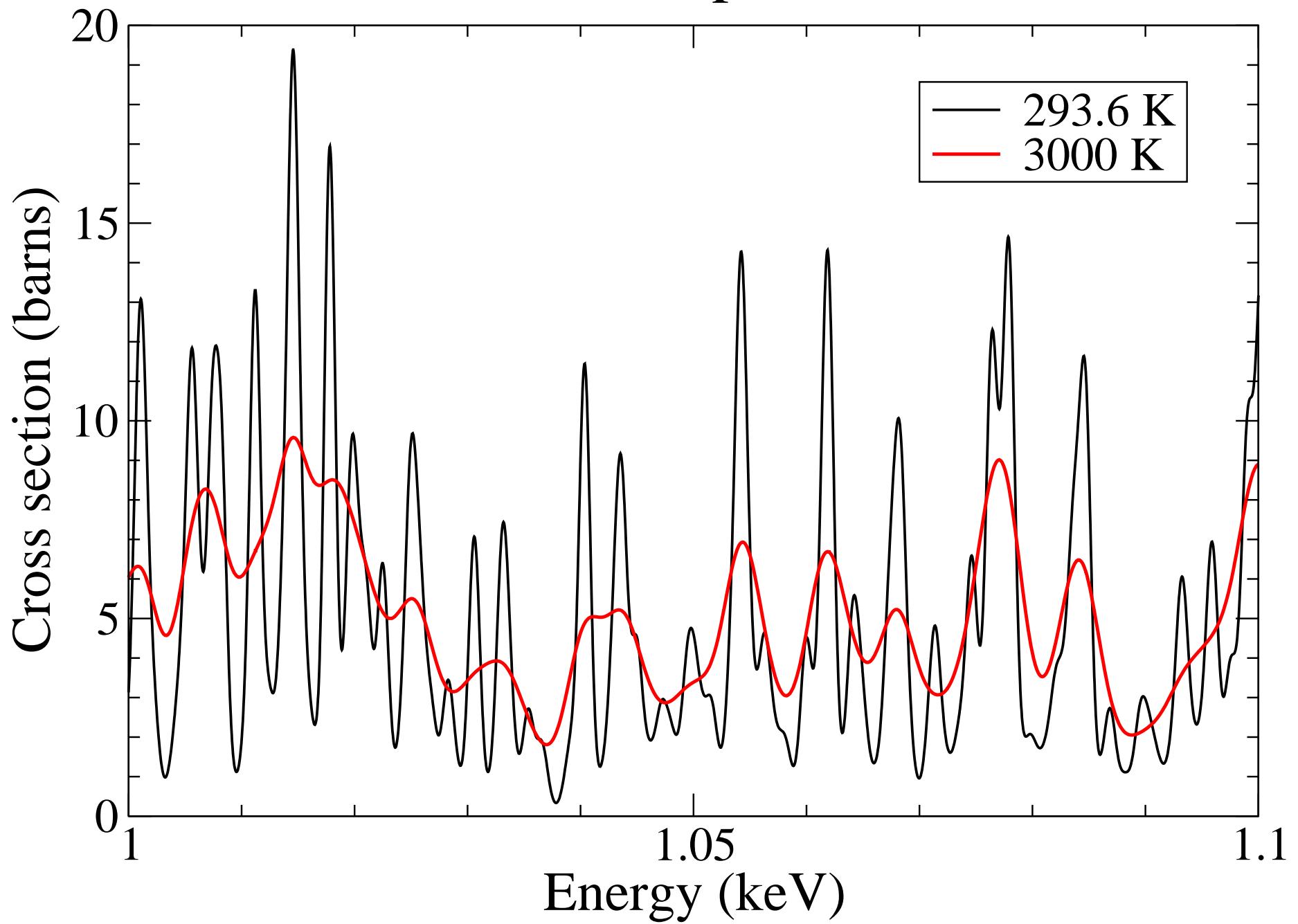
Pu-239 at 2.5 KeV: Points - PT: Line - Infinite Dilute Average



Thermal Issues — I

- Target nuclei are in motion because of non-zero material temperature (assume isotropic Maxwellian).
- Cross sections are Doppler broadened.
- Elastic cross sections can be transformed by a simple model: the free-gas treatment.
- Inelastic cross sections are not subject to this model.

U-235 Absorption Cross Section at two temperatures



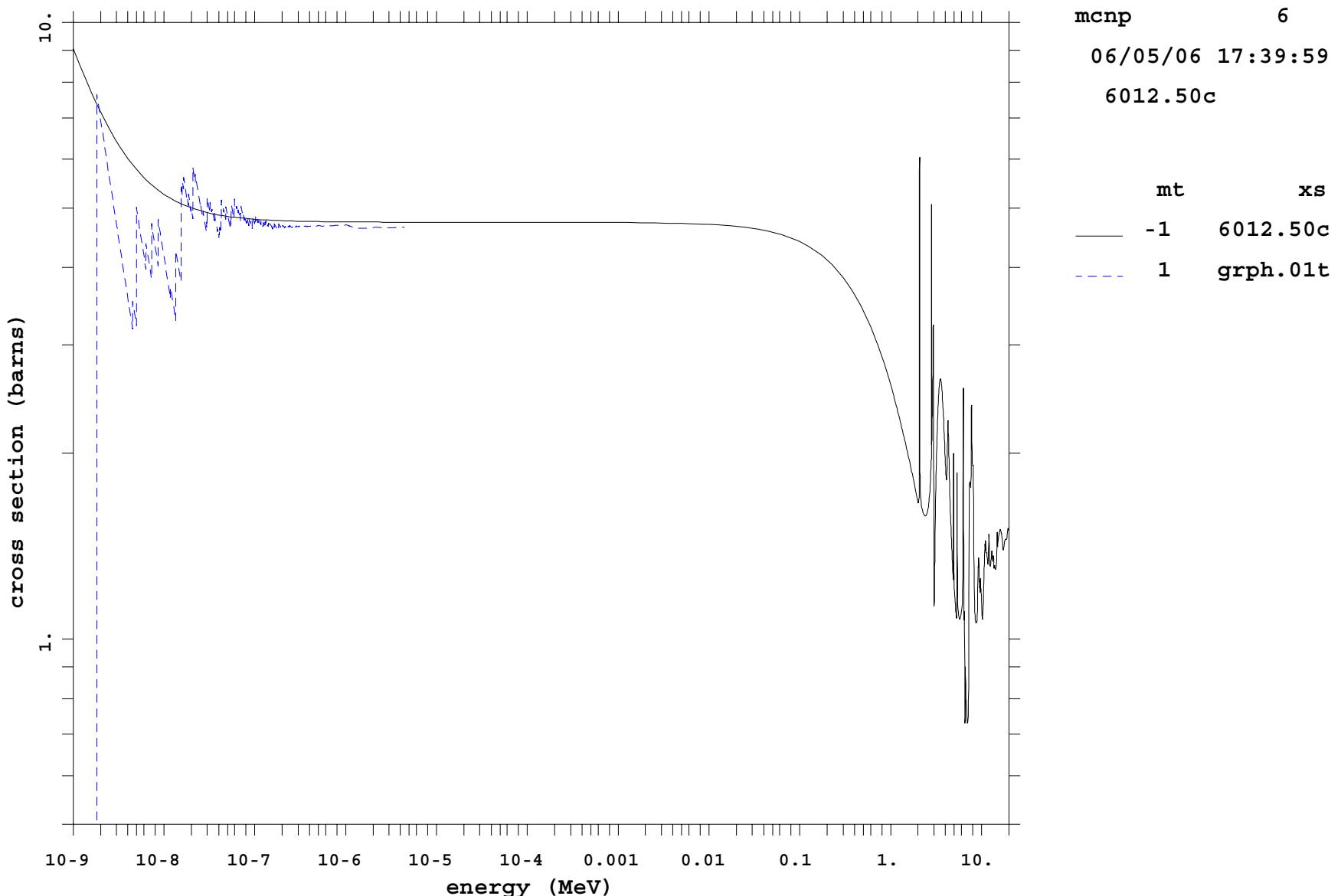
•	92235.11c	233.025000	endf62mt	696398	6.6354E-09	(77 K)
•	92235.12c	233.025000	endf62mt	411854	3.4469E-08	(400 K)
•	92235.13c	233.025000	endf62mt	379726	4.3087E-08	(500 K)
•	92235.14c	233.025000	endf62mt	353678	5.1704E-08	(600 K)
•	92235.15c	233.025000	endf62mt	316622	6.8939E-08	(800 K)
•	92235.16c	233.025000	endf62mt	300278	7.7556E-08	(900 K)
•	92235.17c	233.025000	endf62mt	269062	1.0341E-07	(1200 K)
•	92235.42c	233.024766	endl92	72790	2.5860E-08	(300 K)
•	92235.49c	233.025000	uresa	647347	2.5852E-08	(300 K) ptable
•	92235.50c	233.025000	rmccs	60489	2.5300E-08	(294 K)
•	92235.52c	233.025000	endf5mt	65286	5.0600E-08	(587 K)
•	92235.53c	233.025000	endf5mt	36120	5.0600E-08	(587 K)
•	92235.54c	233.025000	endf5mt	36008	7.5900E-08	(881 K)
•	92235.60c	233.025000	endf60	289975	2.5300E-08	(294 K)
•	92235.61c	233.025000	endf6dn	294963	2.5300E-08	(294 K)
•	92235.64c	233.025000	endf66d	1115810	6.6354E-09	(77 K) ptable
•	92235.65c	233.025000	endf66e	332639	2.5852E-07	(3000 K) ptable
•	92235.66c	233.025000	endf66c	722105	2.5301E-08	(294 K) ptable
•	92235.67c	233.025000	t16_2003	1119233	6.6354E-09	(77 K) ptable
•	92235.68c	233.025000	t16_2003	337079	2.5852E-07	(3000 K) ptable
•	92235.69c	233.025000	t16_2003	726320	2.5301E-08	(294 K) ptable

Thermal Issues — II

- At very low energies (below a few eV), more complex effects become important:
 - Molecular binding energies
 - Vibrational and rotational levels
 - Lattice spacing and crystal structure
- $S(\alpha,\beta)$ data sets attempt to address these issues
 - Replace standard XS below 4 eV
 - Scattering matrix
 - Inelastic and (some) elastic cross sections
 - Correlated in scattered energy and angle

Effect of S(alpha,beta) Tables

s(a,b) total cross section



S(α , b) Sets

- **Beryllium metal:** 77, 294, 400, 600, 800, 1000, 1200 K
- **Benzene:** 294, 400, 500, 600, 800 K
- **Beryllium oxide:** 294, 400, 600, 800, 1000, 1200 K
- **Ortho deuterium:** 19, 20 K
- **Para deuterium:** 19, 20 K
- **Graphite:** 294, 400, 600, 800, 1000, 1200, 1600, 2000 K
- **Hydrogen in Zirconium hydride:** 294, 400, 600, 800, 1000, 1200 K
- **Ortho hydrogen:** 19, 20, 21, 22, 23, 24, 25 K
- **Para hydrogen:** 19, 20, 21, 22, 23, 24, 25 K
- **Deuterium in heavy water:** 294, 400, 500, 600, 800, 1000 K
- **Hydrogen in liquid methane:** 100 K
- **Hydrogen in light water:** 294, 400, 500, 600, 800, 1000 K
- **Hydrogen in polyethylene:** 294 K
- **Hydrogen in solid methane:** 22 K
- **Zirconium in zirconium hydride:** 294, 400, 600, 800, 1000, 1200 K

- Convert cross-section libraries:
 - From Type-1 (ASCII) to Type-2 (binary)
 - From Type-2 (binary) to Type-1 (ASCII)
- Copy entire libraries to new files, Type-1 or Type-2
- Copy selected nuclide table-sets to new libraries, Type-1 or Type-2
- 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(alpha,beta) thermal data to new T
- Create new *xsdir* file which includes all of the above changes

- Taken from "doppler" code by MacFarlane, taken from NJOY
 - References:
 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 Broadening
 - 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(alpha,beta) thermal data or unresolved resonance probability table data
 - Must have existing datasets at BOTH lower & higher temperature

Delayed Neutrons from Fission

- **MCNP4B and earlier**

- multiplicity of neutrons from fission (n_{ubar}) can be either prompt or total
- in both cases energy spectra are those from prompt neutrons and all fission neutrons are produced instantaneously

- **MCNP4C, MCNPX, and later**

- sample each fission neutron as either prompt or delayed
- if prompt, sample for secondary energy as in 4B
- if delayed, sample appropriate delayed spectra (both in time and energy)

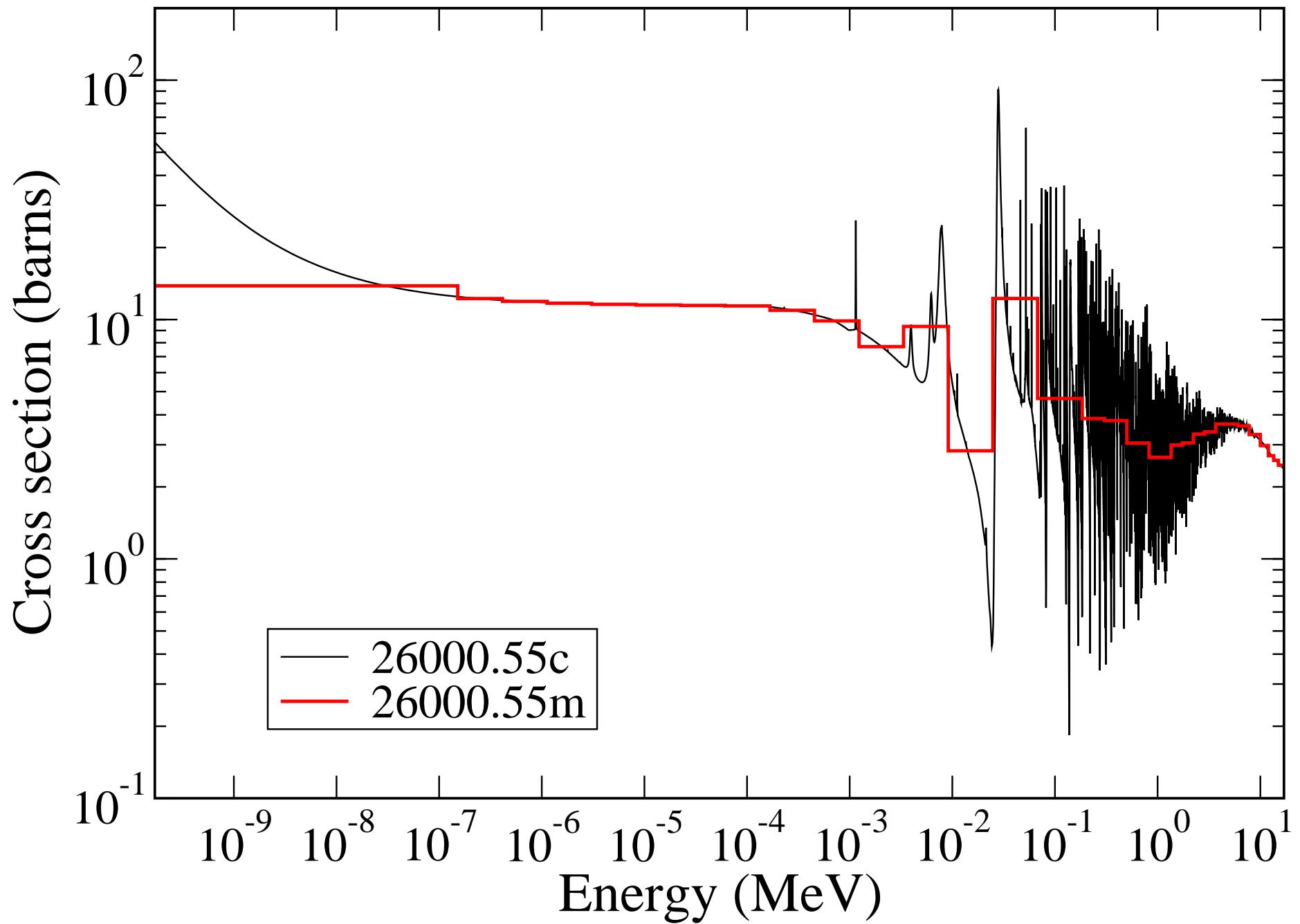
Fission Neutron Multiplicity

- Earlier MCNP/X
 - n = one of two nearest integers to v .
 - For example if $v = 2.43$, only 2 or 3 neutrons would be emitted.
- Recent MCNPX and MCNP, version 1.40:
 - Fission neutron multiplicities can be sampled from a Gaussian distribution.
 - Gaussian width can be user-selected, or set for each isotope from theoretical work by Terrell.
 - More recent predictions of the Gaussian width by Lestone and LANL collaborators are also available

Multigroup Tables

- Cross sections averaged over energy groups.
- Much detail is lost.
- Highly problem-dependent.
- May be needed for
 - Adjoint calculations;
 - Generation of adjoint importance functions;
 - Using the Boltzmann-Fokker-Planck algorithm (charged particles);
 - Comparisons with deterministic transport codes;
 - Applications with missing continuous-energy data.

Continuous-Energy and Multigroup Cross Sections for Natural Iron



Dosimetry Tables

- Incomplete: cannot be used as transport tables.
- Contain (energy, cross section) pairs for various specific reactions.
- Are intended to be used to calculate reaction rates.
- Often provided for reactions used in neutron activation or neutron dosimetry applications
 - for example: $^{46}\text{Ti}(\text{n},\text{p})$ $^{63}\text{Cu}(\text{n},\alpha)$.
- Data sets available from ENDF/B-V and LLNL.
- 463 isotopes of 82 elements from Z = 1 to Z = 98.

Continuous-energy Nuclear Data Libraries



Library	Issued	Source	Identifiers	Total Nuclides	Nuclides with Probability Tables for Unresolved Resonance Region	Fissioning Nuclides with Delayed-Neutron Spectra
ENDF60	1994	ENDF/B-VI.2	.60c	122	0	0
ENDF66	2002	ENDF/B-VI.6	.64c, .65c, .66c	173	67	22
ACTI	2002	ENDF/B-VI.8	.61c, .62c, .63c	41	4	0
T16_2003	2004	LANL T-16	.67c, .69c, .68c	15	13	14

77 K

293 K

3000 K

- The final release of ENDF/B-VI, ENDF/B-VI.8, was distributed in October 2001
- ACTI can be combined with ENDF66 to produce a nuclear data library that corresponds to the final release of ENDF/B-VI for almost all nuclides
- The combination of ACTI and ENDF66 hereafter will be referred to as ENDF/B-VI
- T16_2003 was developed by LANL nuclear physics group (T-16)
- T16_2003 contains data for ^3H , the uranium isotopes, ^{237}Np , ^{239}Pu , ^{241}Am , and ^{243}Am
- The most notable changes in T16_2003 involve inelastic and elastic scattering cross sections, fission spectra, and the average number of neutrons emitted per fission.
- **ENDF60, ENDF66, ACTI, and T16_2003 are included in the MCNP5 distributions from RSICC.**

- **SAB2002, a library of thermal scattering laws $S(\alpha,\beta)$, was released in 2002**
- Data in SAB2002 are derived from ENDF/B-VI (ENDF/B-VI.3)
- SAB2002 contains data for 15 combinations of nuclides and materials
- Typical temperature ranges are from 294 K to 1200 K, in increments of 200
- Data typically are tabulated at 16 angles and 64 energies for each temperature
- Data are provided at ~ 20 K for a limited number of nuclides
- **SAB2002 is included in the MCNP5 distribution from RSICC**

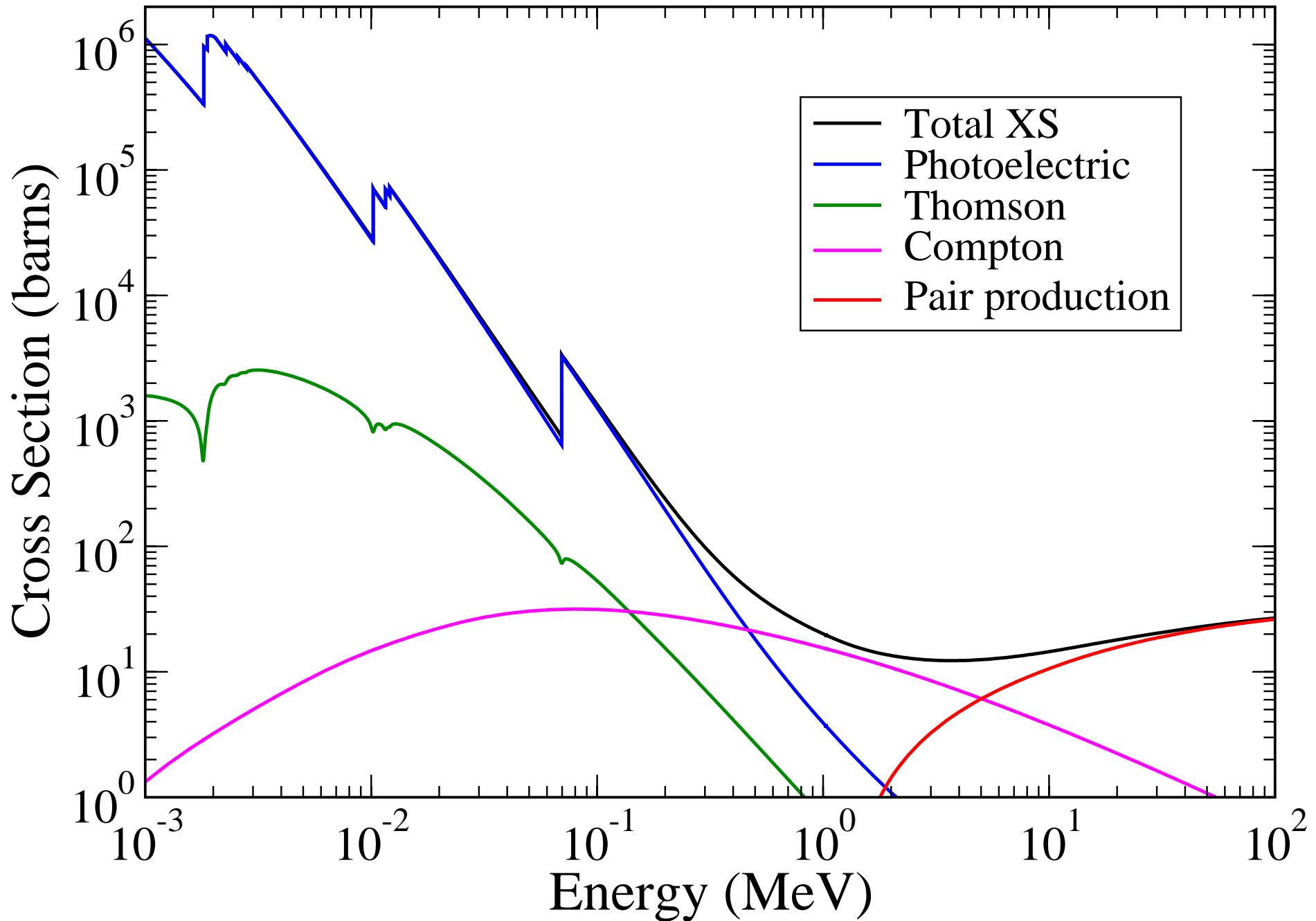
Some selected neutron approximations

- Each secondary particle from neutron collision sampled independently.
- Neutron reaction and photon-production reaction not correlated.
- No delayed photon production (about half of fission gamma energy).
- Only approximate treatment of thermal effects.
- No direction-dependent crystal effects.
- No charged-particle production above α .
- Linear Monte Carlo only.
- Cross sections are inherently uncertain.

Photo-atomic Transport Tables

- Continuous energy representation.
- Four photon processes:
 - Coherent (Thomson) scattering with form factors.
 - Incoherent (Compton) scattering with form factors,
 - now including Compton “Doppler” broadening.
 - Photoelectric absorption with atomic relaxation.
 - Pair production
- Thick-target bremsstrahlung approximation available.
- Energy range 1 keV to 100 GeV.

Photon Cross Sections in Tungsten



Doppler Energy Broadening for Photons

- Incoherent photon scattering can occur with a bound electron and generate a Compton electron and a scattered photon
 - The electron binding effect becomes increasingly important for incident photon energies less than 1 MeV
- The bound-electron *effect on the angular distribution* of the scattered photon appears as a *reduction of the total scattering cross section* in the forward direction
 - This effect has been accounted for in MCNP by modifying the Klein-Nishina cross section with a form factor
- The bound-electron *effect on the energy distribution* of the scattered photon appears as a *broadening of the energy spectrum* due to the pre-collision momentum of the electron
 - This second effect is *the definition of Doppler energy broadening* for incoherent photon scattering and is new in MCNP 5

Doppler Energy Broadening for Photons

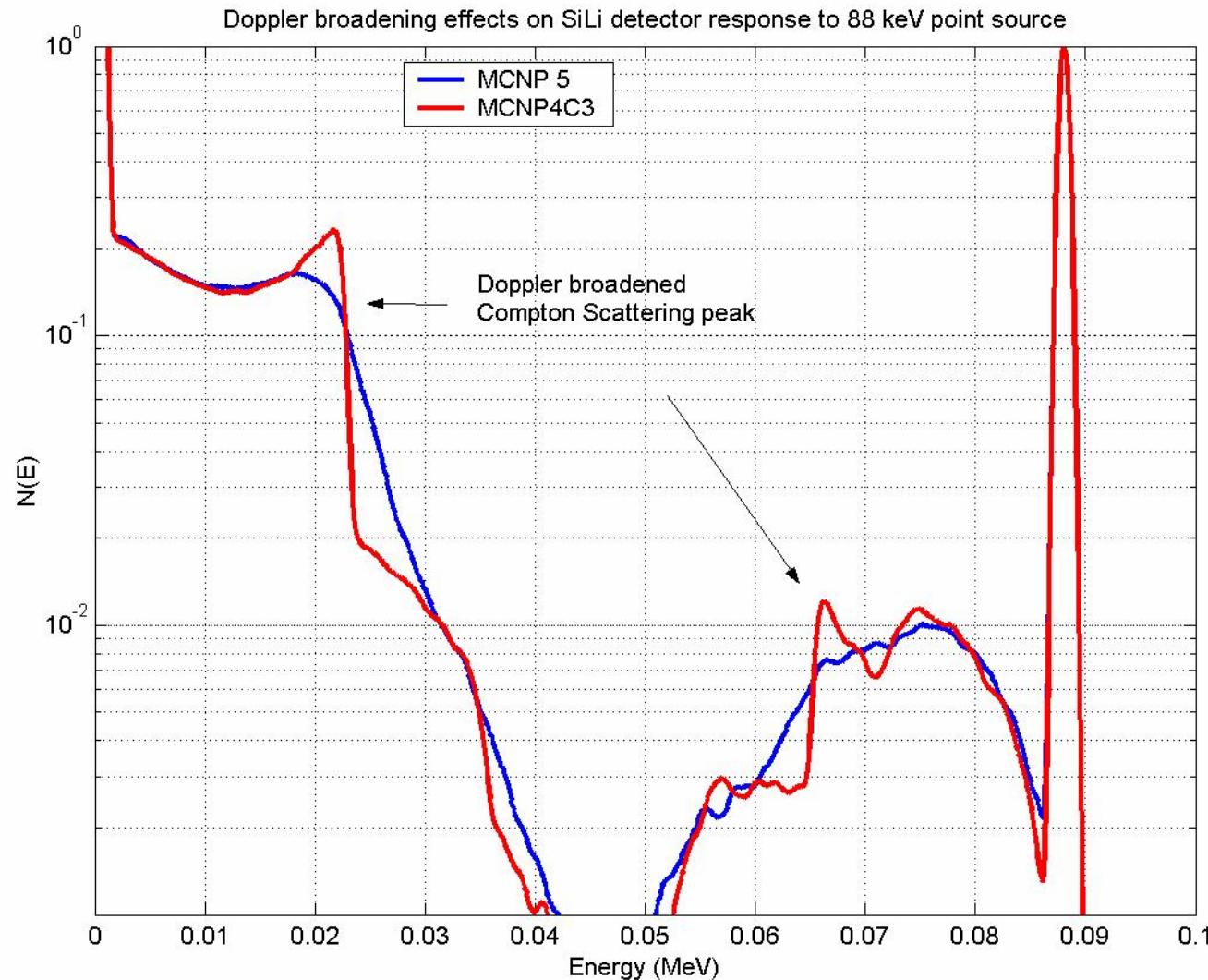


Photo-nuclear Reaction Tables

- Cross-section and production data for neutrons and for light isotopes:
 - Protons, Deuterons, Tritons, ^3He , and ^4He (α).
- LANL evaluations include 13 isotopes:
 - ^2H , ^{12}C , ^{16}O , ^{27}Al , ^{28}Si , ^{40}Ca , ^{56}Fe , ^{63}Cu , ^{181}Ta , ^{184}W , ^{206}Pb , ^{207}Pb , and ^{208}Pb .
- IAEA Evaluated Photonuclear Library includes 164 isotopes of 48 elements.
 - <http://t2.lanl.gov/data/photonuclear.html>
- ENDF tables will be extended with ENDF/B-VII.

Some selected photon approximations

- No thermal effects.
- No molecular binding or solid state effects.
- Only K and L edges treated in photoelectric absorption and atomic relaxation.
- No anomalous scattering factors
- No distinction between pair and triplet production.
- No treatment of polarization.
- No photonuclear production above α .
- Thick-target bremsstrahlung is a rough approximation.

Electron Transport

- Based on hybrid Class I algorithm of the ETRAN series of codes, particularly the Integrated TIGER Series (without the PCODES or MCODES options).
- Data are provided for secondary particle production:
 - Bremsstrahlung
 - Knock-on electrons
 - Characteristic X-rays and Auger electrons.
- Photons from positron annihilation are followed.
- Collisional processes for energy loss and angular deflection are modeled.

Energy loss and angular deflection

- Mean energy loss from Bethe-Bloch theory combined with the Møller cross section (through Berger).
- Density-effect corrections from Sternheimer, Berger, and Seltzer.
- Energy loss straggling from Landau theory with enhancements from Blunck, Leisegang, Westphal, and Seltzer.
- Angular deflection from Goudsmit/Saunderson theory.

Recent Electron Improvements

- Data-related improvements (EL03 data libraries):
 - Radiative stopping powers;
 - Density effect corrections;
 - Electron-induced X-rays;
 - Bremsstrahlung production;
 - Variance reduction.
- Detailed Landau straggling logic.
 - Steps toward eliminating cell-size artifacts.

Selected electron approximations

- No thermal, molecular binding, or solid state effects.
- Class I condensed history model.
- Only K and L atomic relaxation.
- Electron-induced characteristic X-rays are only from the highest-Z component of a material.
- No electric or magnetic fields for electrons.
- No effects of charge buildup on transport.
- Positrons annihilate at rest.
- Low-energy electron cross sections are very uncertain.

Proton Transport Tables

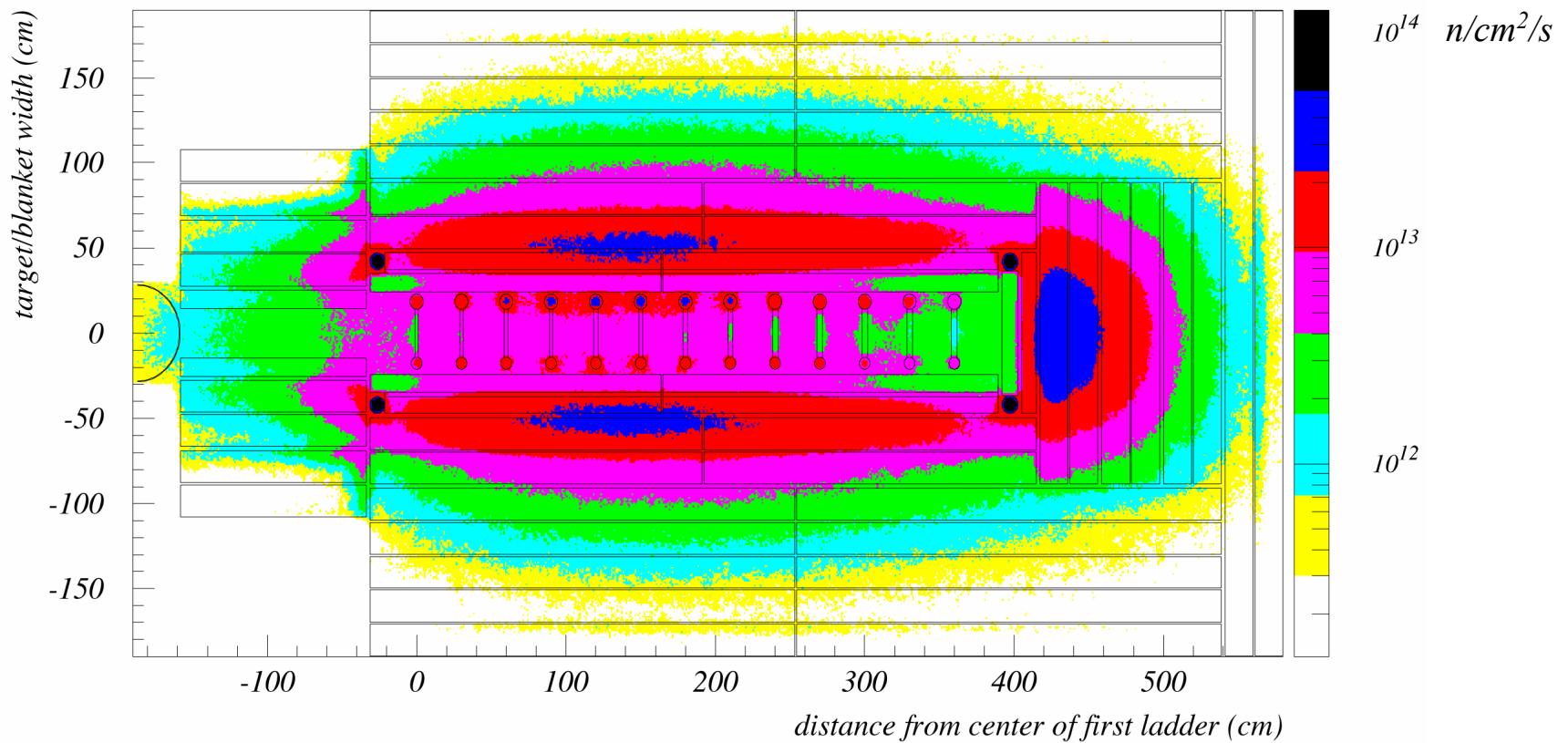
- Developed using the GNASH code system.
- Energy range 1 – 150 MeV.
- Evaluations include:
 - Total, nuclear elastic plus interference, and inelastic cross sections.
 - Production cross sections for neutrons, protons, deuterons, tritons, ^3He , ^4He , photons, and heavy recoils.
 - Double-differential production spectra for neutrons, protons, deuterons, tritons, ^3He , and ^4He .
 - Angle-integrated emission spectra for photons and heavy recoils.

Initial Release: LA150H

- Full ENDF-VI-format evaluations for 42 isotopes:
 ^1H , ^2H , ^7Li , ^{12}C , ^{14}N , ^{16}O , ^{27}Al , ^{28}Si , ^{29}Si , ^{30}Si , ^{31}P , ^{40}Ca ,
 ^{50}Cr , ^{52}Cr , ^{53}Cr , ^{54}Cr , ^{54}Fe , ^{56}Fe , ^{57}Fe , ^{58}Ni , ^{60}Ni , ^{61}Ni , ^{62}Ni ,
 ^{64}Ni , ^{63}Cu , ^{65}Cu , ^{93}Nb , ^{182}W , ^{183}W , ^{184}W , ^{186}W , ^{196}Hg , ^{198}Hg ,
 ^{199}Hg , ^{200}Hg , ^{201}Hg , ^{202}Hg , ^{204}Hg , ^{206}Pb , ^{207}Pb , ^{208}Pb , and ^{209}Bi .
- This set will be extended in ENDF-VII.

- Current release candidate is ENDF/B-VII β -2, which had an informal release in April, 2006
 - 393 incident neutron evaluations (many new)
 - 20 thermal S(alpha, beta) evaluations (some new)
 - 163 photonuclear evaluations (new sublibrary)
 - total of 58 evaluations for incident protons, deuterons, tritons, and He-3 (updated and extended)
 - note that the photoatomic data was not updated from ENDF/B-VI.8
 - Relative to ENDF/B-VI, the changes to the data for the actinides are similar to those incorporated into T16_2003 but are more extensive
 - The cross sections for ^{233}U , ^{235}U , and ^{238}U incorporate revised resonance data from Oak Ridge National Laboratory
 - Cross sections for ^1H and ^{16}O also have been revised
 - Changes for other nuclides are too numerous to discuss here
- CSEWG will meet at Brookhaven in late June, 2006, to discuss benchmark testing results and any last issues
- CSEWG currently plans to release the initial version of ENDF/B-VII in late summer 2006

APT: Neutron flux in the target region



APT: Neutron flux in an RF line

