NJOY-2005
New Structure and Features

R.E.MacFarlane
Los Alamos National Laboratory

- NJOY-2005 is a translation of NJOY99 to Fortran-90/95 style using a modern modular structure and an extended code-management scheme.
- There are new features for resonance reconstruction, MCNP thermal scattering, plotting of MCNP tallies, and preparing data in the Los Alamos NDI format.

What is NJOY?

- NJOY is a comprehensive nuclear data processing system designed to convert physics data in the Evaluated Nuclear Data Files (ENDF) format into forms useful for nuclear applications.
- It is widely used to prepare data for particle transport codes using both multigroup and Monte Carlo (MCNP) methods. It has supported applications in fusion and fission reactor work, weapons, criticality safety, radiation shielding, medicine, accelerators, materials science, and space travel.
- The code also makes some physics additions to the basic ENDF data, including radiation heating and damage, gas production, and thermal scattering from liquid and solid moderator materials.
- NJOY is also useful for supporting data work, both experiment and evaluation, through the analysis of experiments, plotting, and sensitivity studies.

Why Fortran-90/95 Style?

- Using Fortran-90/95 type coding can improve portability, maintainability, and reliability.
- Formal F90 modules are used to encapsulate functions or data and for “information hiding.”
- COMMON blocks are eliminated in favor of global variables encapsulated in modules, which provides for strong typing and protects against some of the side effects where changes in one location cause problems elsewhere.
- The home-grown allocation scheme used to provide variable dimensioning in the F77 version is replaced by allocated arrays, which makes the logic much clearer.
- Variable typing using the KIND system is much more portable than the older methods, and the strong typing that can now be used helps to prevent inappropriate combinations of data types.

More on Fortran-90/95

- Using NO IMPLICIT helps to discipline the programmer and helps to catch problems introduced by changes before they can bite you.
- The CHARACTER data type is more portable than the older “Hollerith” data.
- The need to have many different system-dependent modifications is greatly reduced or completely eliminated.
- Free format lines, a reduction in the use of line numbers, and extensive use of indented block constructs make the code easier to read.

Service Modules

- Moving common utility routines and data values to special service modules helps to clean up the coding:
- The module physics.f90 contains common parameters, such as the Boltzman constant, pi, the speed of light, and the neutron mass that are used all over the program by just saying “use physics.”
- The module endf.f90 contains routines that are used to read and write ENDF data throughout the program.
- The module graph.f90 contains the low-level routines that enable NJOY to prepare graphs in Postscript format.
- The module util.f90 contains things like the time and date calls.
- The module mathm.f90 exports math routines, such as erfc, gami, and legndr. Subsidiary routines used in generating these values are hidden by the module structure and not accessible from outside the module.
- Others include locale.f90, version.f90, and samm.f90.

The Main Modules

- The main components of NJOY, which we always called “modules,” are now implemented as F90 modules: the module reconr.f90 does resonance reconstruction, broadr.f90 does Doppler broadening, etc.
- The ACER module for preparing MCNP libraries has been split up into a main module acer.f90, the module for preparing normal class “c” files (acefc.f90), the module for preparing thermal class “t” data (aceth.f90), and so on. The module acecm.f90 contains common routines used by other ACER subsidiary modules.
- There is another subsidiary module, samm.f90. It Implements the SAMMY methods of resonance reconstruction, and it can be used by either RECONR or ERRORR.
- There are also the new modules ndir.f90 for preparing Los Alamos NDI interface data, and tallyr.f90 for interfacting MCNP tallies to the NJOY plotting system.

Portability

- The F90 version of NJOY has been tested on a wide variety of systems including Sun, linux, Windows PC, and Mac OS X, with compilers from Sun, Absoft, Intel, IBM, Lahey, and GNU.
- Lately, we've been concentrating on g95, because it is free, available for all systems, and works well. The g95 compiler is very strict about Hollerith data and required changes in the codes that were not needed on the other systems. It also requires DEALLOCATE statements when leaving subroutines that other systems don't.

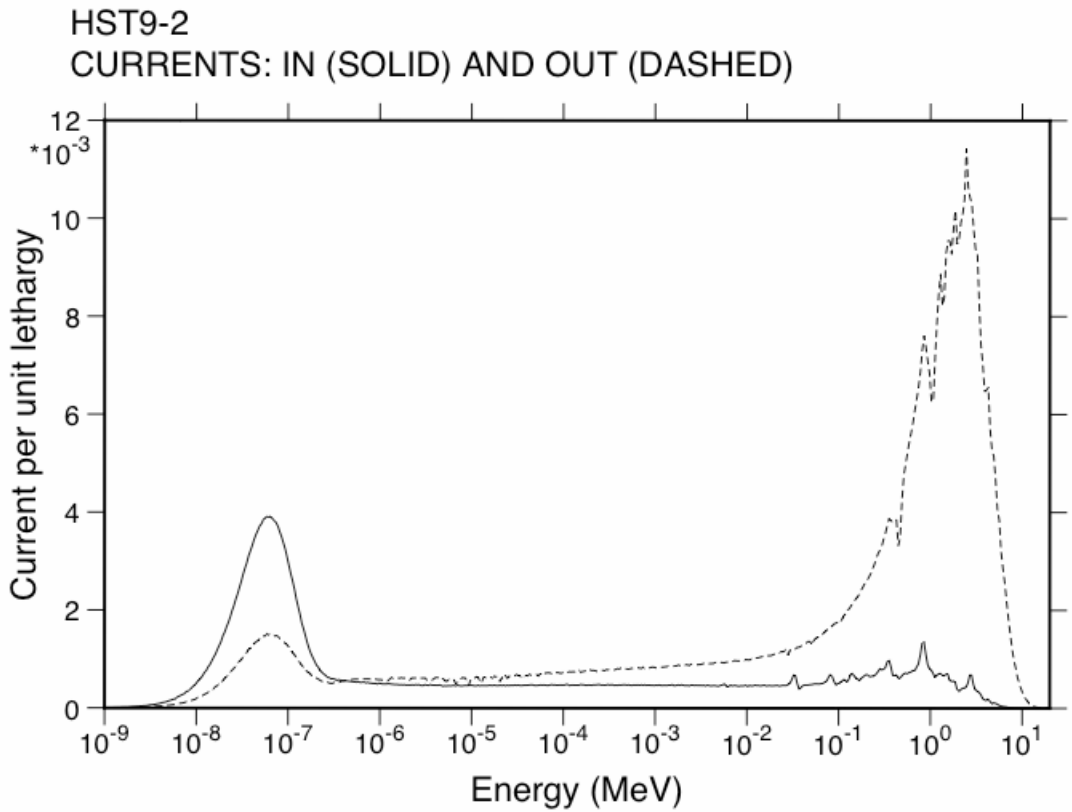
Code Maintenance

- Code maintenance is a very important part of modern QA procedures. It will be discussed in the companion talk on TRANSX-2005.
- Changes have been made to our existing UPD code to handle free format F90 lines where our classical line identifiers cannot be used, to maintain both the code and the manual in the same context, and to make it easier to make changes by editing the code directly and then generating the differences for the code history file.

The TALLYR Module

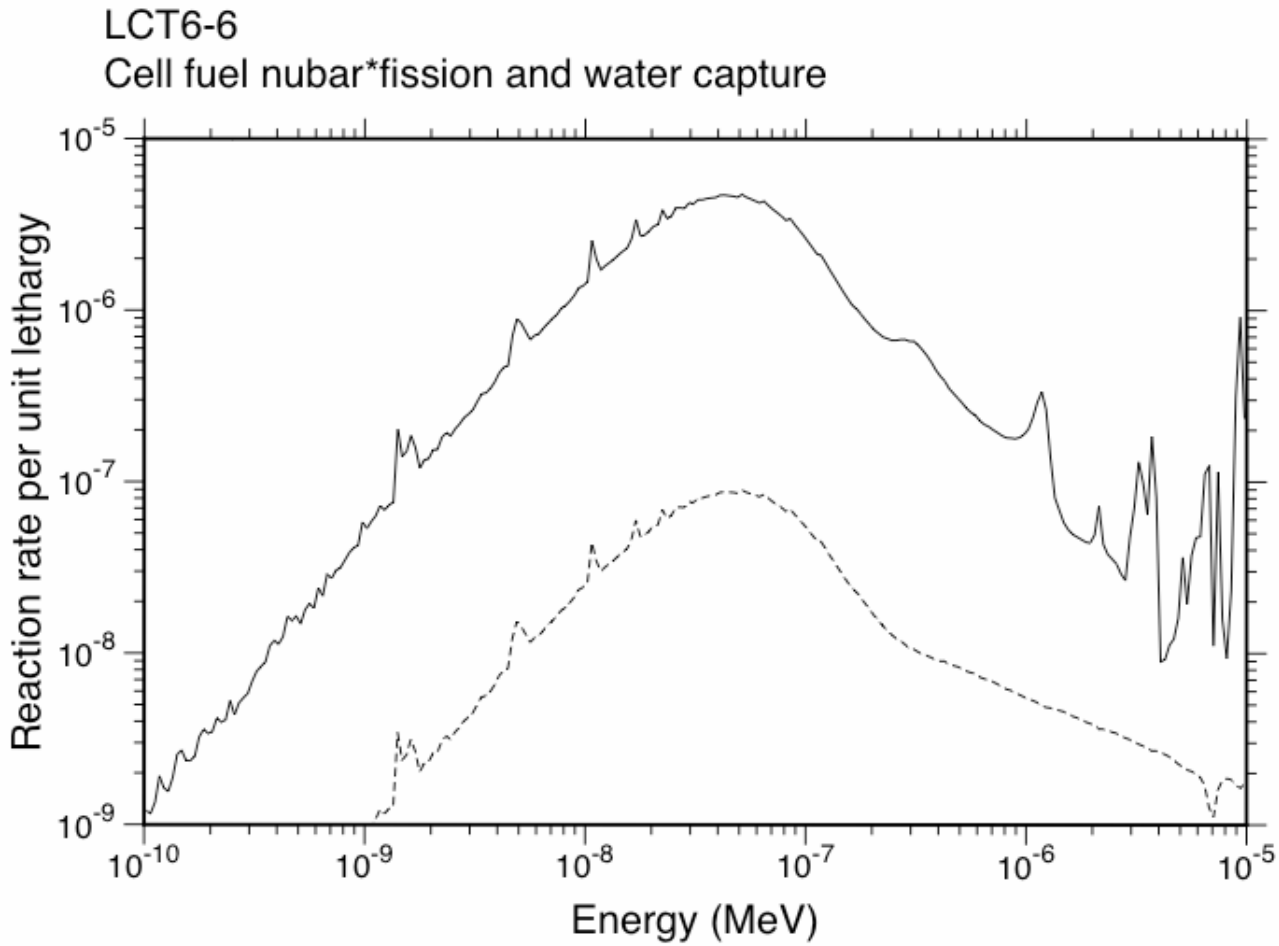
- N JOY is very closely connected to MCNP both by history and in practice. Some MCNP users have had to become NJOY users to prepare their own data. Those who know both codes may like the new TALLYR module.
- This module can read in MCNP output listings, extract selected tallies, and plot them as Postscript graphs with all the nice features of NJOY graphics. Different tallies can be compared by plotting them both on a page, or by plotting the ratio, percent difference, or actual difference between the curves. Data can be plotted per unit lethargy, per unit energy, as a cumulative integral, or transformed in several ways,
- Data points can be plotted with MCNP error bars, or shaded error corridors can be requested instead.

A TALLYR Example



MCNP Thermal Treatment

- The current MCNP treatment for bound thermal scattering was developed in the mid 80's when computers were much smaller than today. The scattering for each incident energy is represented by a set of equally probable discrete cosines and a set of discrete emitted energies on a predefined probability grid. The tmccs set of earlier MCNP releases used 8x20 for this sampling. The current sab2002 set of MCNP5 uses 16x64 discrete events.
- This approach was designed to give reasonable values for the integrals over cross sections that are important for criticality. It clearly is lacking for problems dominated by first collisions and problems with very fine detector energy or angle resolution.

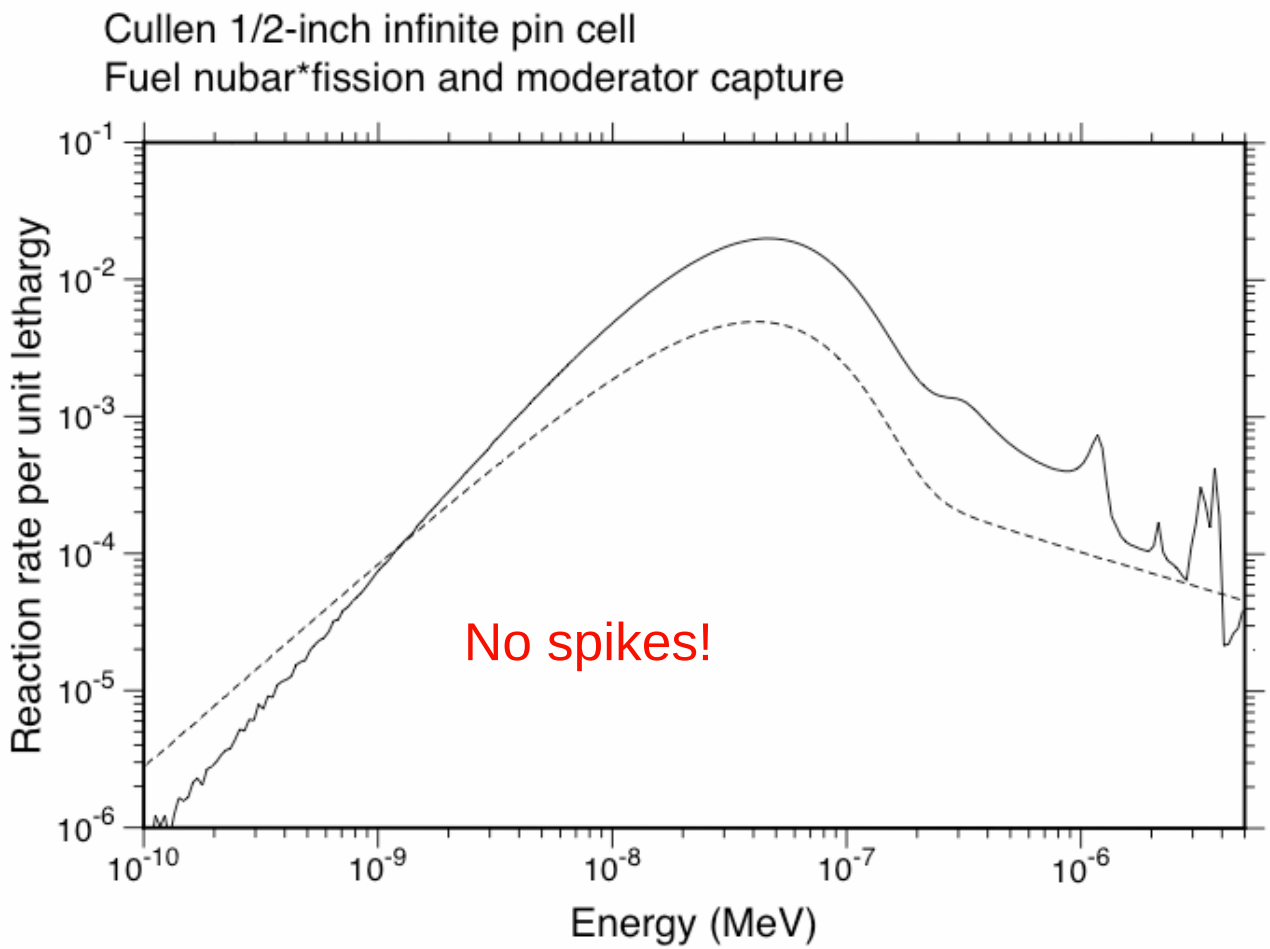

LCT6-6
Cell fuel nubar*fission and water capture
Reaction rate per unit lethargy
10-5
10-6
10-7
10-8
10-9
10-10
10-9
10-8
10-7
10-6
10-5
Energy (MeV)

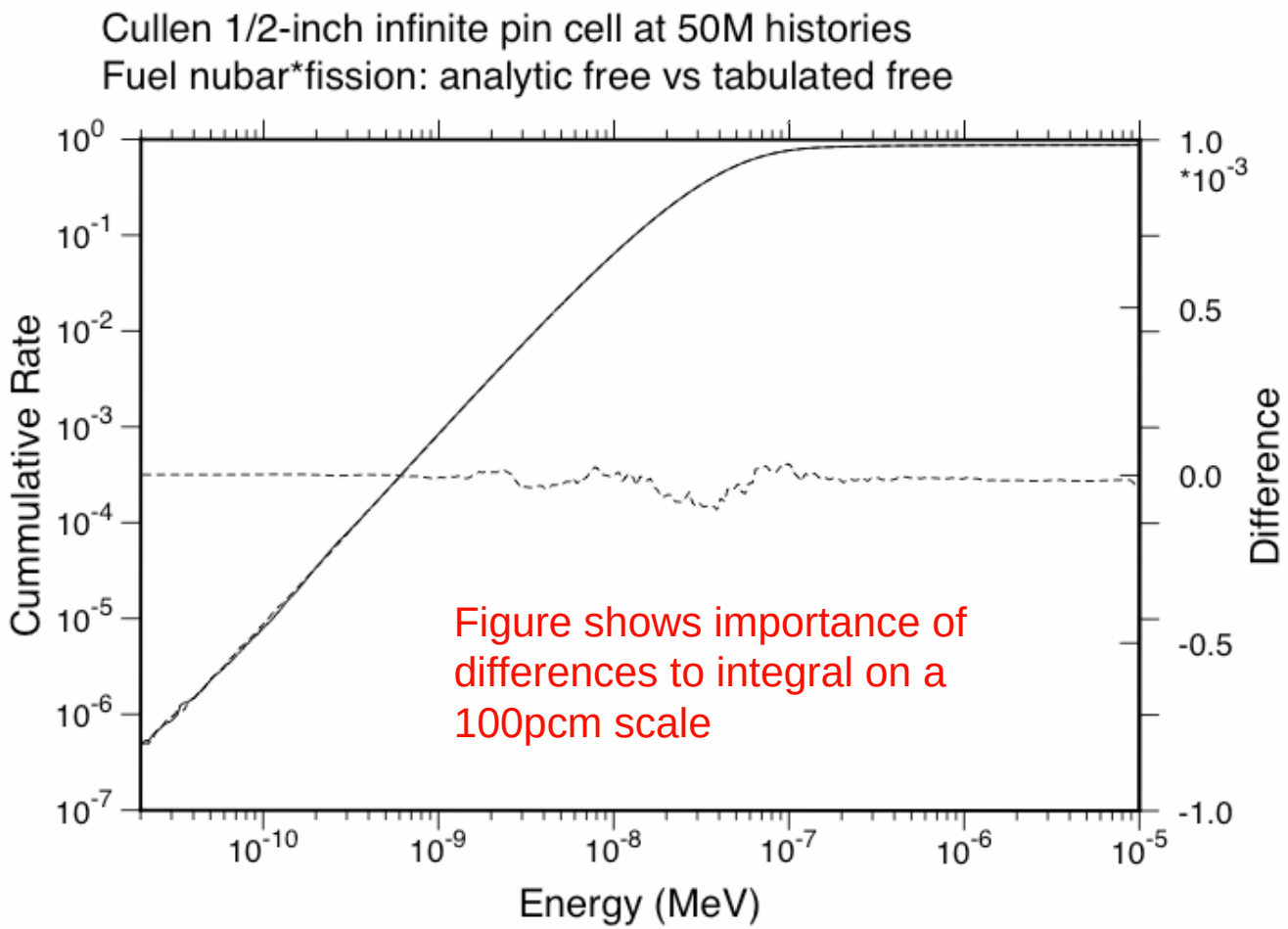
Continuous Tabulated Method

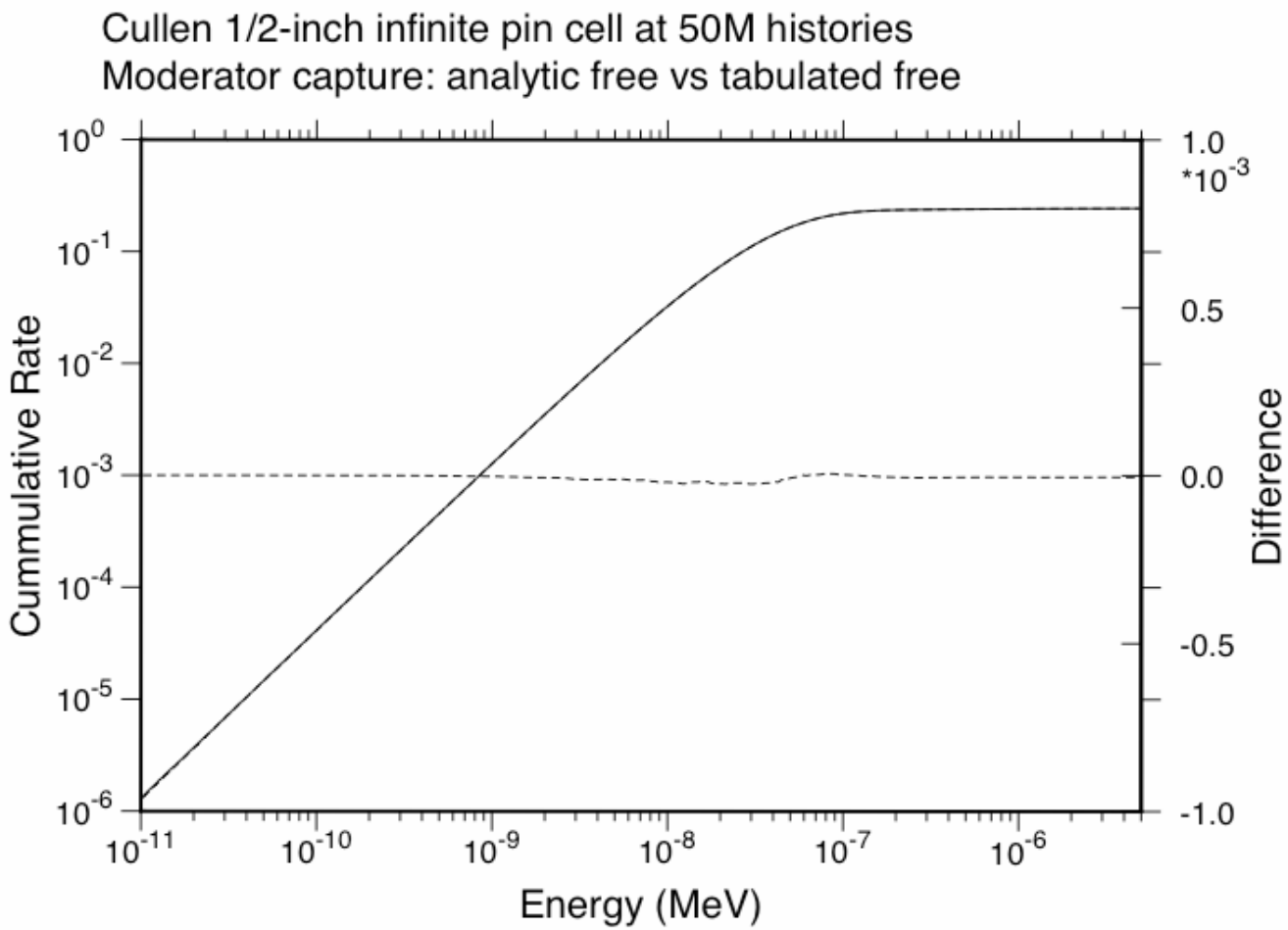
- To get rid of these offensive “spikes”, we developed a new continuous tabulated method for thermal sampling in MCNP. The continuous spectra already available from THERMR are converted to the pdf/cdf form used for sampling other distributions in MCNP. The normal equally probable cosines from THERMR are still given in the new version of the ACE file.
- The sabcol routine of MCNP5 was modified to use the new data for S(alpha,beta) collisions. The pdf/cdf tables are binary searched for each random sample and the cosines are interpolated to the resulting emission energy at the nearest energy grid value to the incident neutron energy. This emission energy is then projected up or down to the actual incident energy with a combination of constant energy transfer (to preserve the E’=E edge and the discrete excitations) and unit base (to avoid problems at lower energies).

CT Method (continued)

- The discrete cosines from the nearest energy grid point are spread out to cover the entire angular range. This can be a little ragged at back angles when the scattering probability gets to be small. The first collision angular performance of this method won't be quite as smooth as its energy performance.
- We have tested this new method by constructing continuous tabulated data from the free-gas hydrogen S(alpha,beta) using all our standard methods and comparing the results to the analytic free gas model built into MCNP. Good results in this comparison should be a reliable indicator of its performance for ordinary criticality calculations.


Cullen 1/2-inch infinite pin cell
Fuel nubar*fission and moderator capture
Reaction rate per unit lethargy
Energy (MeV)
No spikes!


Cullen 1/2-inch infinite pin cell at 50M histories
Fuel nubar*fission: analytic free vs tabulated free
Cummulative Rate
Difference
Energy (MeV)
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
1.0
*10^{-3}
0.5
0.0
-0.5
-1.0
10^{-10}
10^{-9}
10^{-8}
10^{-7}
10^{-6}
10^{-5}
Figure shows importance of differences to integral on a 100pcm scale


Cullen 1/2-inch infinite pin cell at 50M histories
Moderator capture: analytic free vs tabulated free
Cummulative Rate
Difference
Energy (MeV)
10^0
10^-1
10^-2
10^-3
10^-4
10^-5
10^-6
1.0
*10^-3
0.5
0.0
-0.5
-1.0
10^-11
10^-10
10^-9
10^-8
10^-7
10^-6

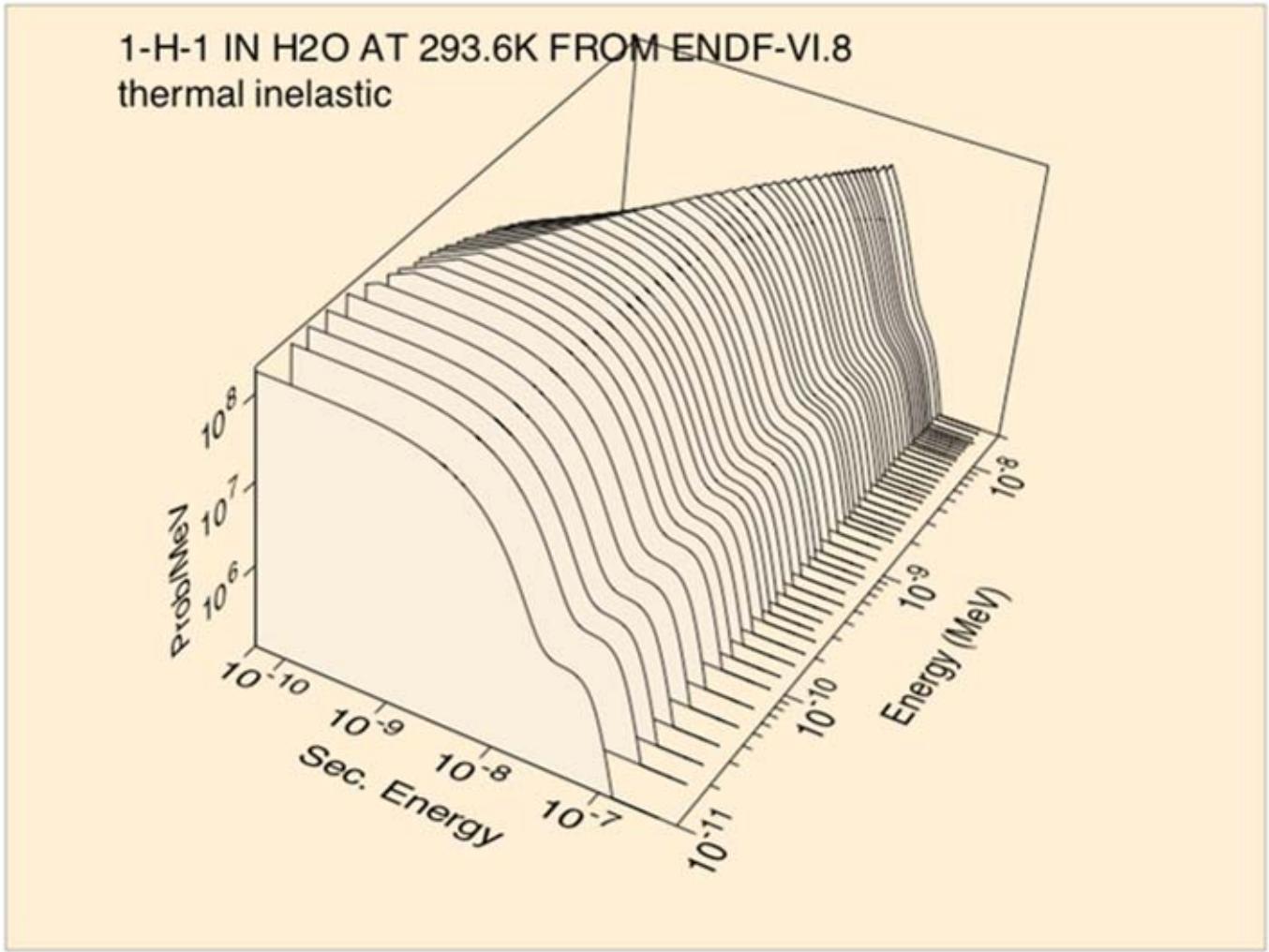
Integral Performance

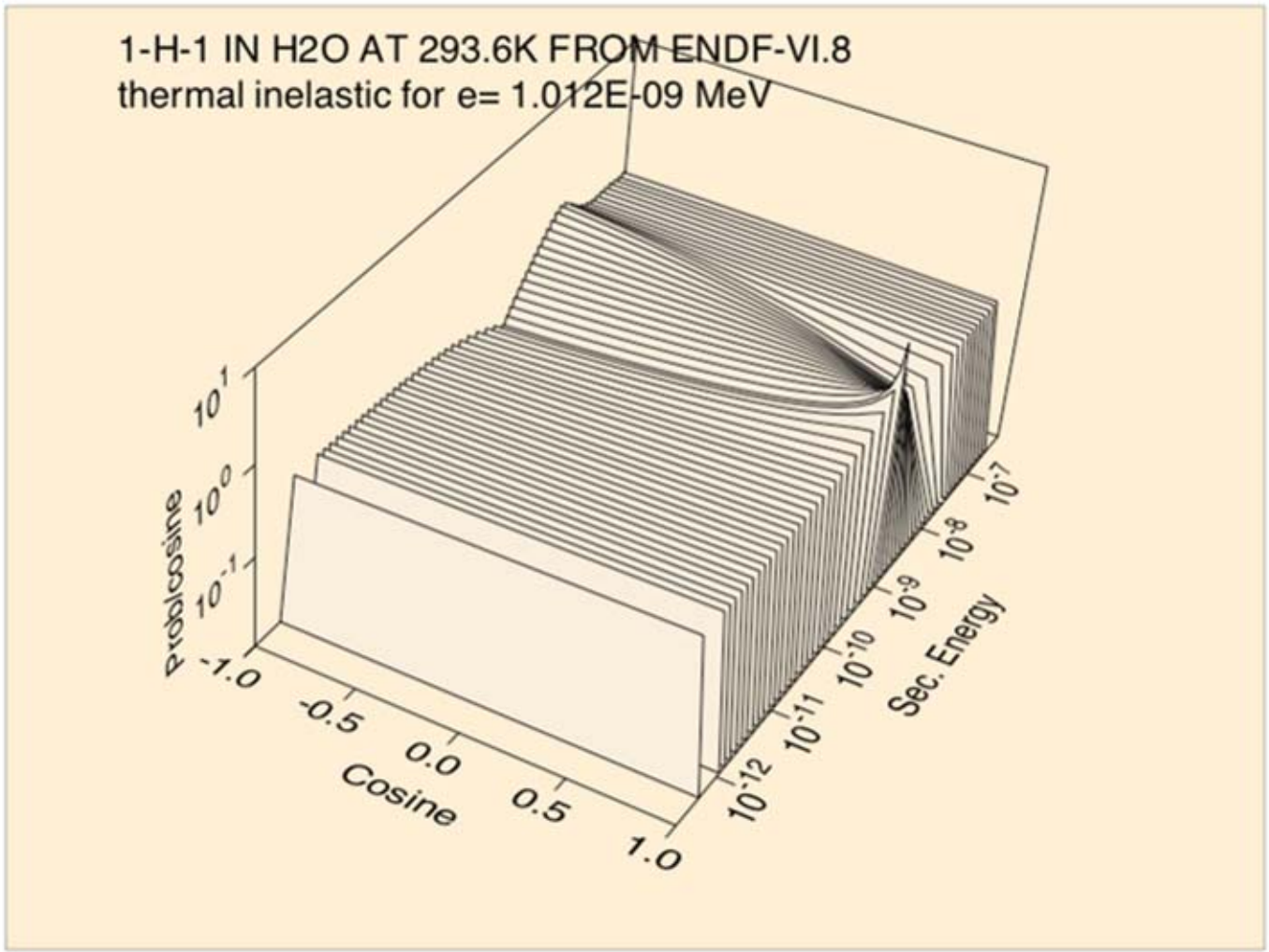
- It should be stressed that the existing MCNP5 methods and data perform well for normal thermal critical assembly calculations. This new method is desirable in following the MCNP dictum of having the best physical representations possible, but existing users should not be too concerned about the validity of their work.

Assembly	Discrete	Continuous
LCT6-6	0.99935(22)	0.99910(26)
HST9-2	1.00061(22)	1.00079(22)

Thermal Plotting

- The new ACER coding to support the continuous tabulated method also makes more extensive plots of the thermal data. In addition to the previous cross section, mubar, and ebar plots, we have 3-D views of the energy distributions and 3-D views of the energy-angle distributions.


1-H-1 IN H2O AT 293.6K FROM ENDF-VI.8
thermal inelastic
Prob/MeV
10^8
10^7
10^6
10^-10
10^-9
10^-8
10^-7
Sec. Energy
10^-11
10^-10
10^-9
10^-8
Energy (MeV)


1-H-1 IN H2O AT 293.6K FROM ENDF-VI.8
thermal inelastic for e= 1.012E-09 MeV
Probl cosine
10^1
10^0
10^-1
-1.0
-0.5
0.0
0.5
1.0
Cosine
10^-12
10^-11
10^-10
10^-9
10^-8
10^-7
Sec. Energy

SAMMY Resonance Treatment

- SAMMY is a high quality resonance fitting code developed at Oak Ridge and used for many of the modern resolved resonance evaluations. Recently, they have found reason to extend the ENDF formats to allow for more detailed resonance physics, including charged particle channels, and to represent the complex covariance information produced by SAMMY.
- To help to make these new features available to the community, Nancy Larson has made available some of the resonance coding from SAMMY. We have converted that coding into a F90 module samm.f90 using the NJOY coding style.
- The samm module exports calls that can be used to compute resonance cross sections, angular distributions, and derivatives of the cross sections with respect to the resonance parameters.

SAMMY continued

- The RECONR module of NJOY has been modified to allow the resonance cross sections to be computed using samm routines, if desired. The results have been tested against SAMMY results and verified against an independent installation of the method into Red Cullen's PREPRO system. The capability is now ready to use when new evaluations that require it are prepared.
- A test interface for computing angular distributions from resonance parameters has also been installed in RECONR. At the current time, the angular distributions can be computed and printed, but they are not coupled into the PENDF output for use in subsequent modules. More tests of this capability and additional development are waiting for good test evaluations to become available.

SAMMY Derivatives

- The capability to compute derivatives with respect to resonance parameters has been tested against Nancy's results. In the future, it would be called by the ERRORR module to provide sensitivity functions to be combined with resonance parameter uncertainty data to generate averaged covariance matrices for use in formal sensitivity calculations.

The NDIR Module

- The new NDIR module provides multigroup cross sections in the Los Alamos Nuclear Data Interface (NDI) format. This is a flexible keyword type text format for multigroup data used for large simulation codes at Los Alamos, and other users can safely ignore it.

Validation

- Another important part of a QA plan is validation. NJOY has 15 test problems to verify its installation and to act as examples of its use.
- Since NJOY-2005 evolved from NJOY99, direct comparisons between the two codes were made for a sampling of results, and they appeared to be consistent.
- The new version was used to process all the materials of ENDF/B-VI many of the proposed preVII materials, and many of the materials from JEFF-3.1t with good results. These files were used in test testing runs using both mulitigroup methods and MCNP and then cross compared to earlier results using NJOY99 where possible. The results were consistent.

Status

NJOY-2005 is being packaged for release by June