

The NJOY Nuclear Data Processing System - Current Status and Future Plans

A. C. (Skip) Kahler & R. E. MacFarlane
akahler@lanl.gov

**T-2, Nuclear & Particle Physics,
Astrophysics & Cosmology Group
Theoretical Division
Los Alamos National Laboratory**

***Presented at the OECD/NEA Workshop on
Processing Tools for Evaluated Nuclear Data Libraries***

NJOY - Introduction

- The base version of NJOY99 is distributed by ORNL's RSICC and the NEA Data Bank.
 - Updates are maintained at Los Alamos and distributed freely at <http://t2.lanl.gov/codes/njoy99>.
 - Machine dependent updates and sample makefiles for a variety of compilers and hardware/OS configurations are included here.
 - The current version of the code is 99.259.
 - In-house updates through 99.279 will be posted at the end of November.

- A new base version, NJOY2008, is nearing completion with distribution to ORNL's RSICC anticipated by the end of 2008.

NJOY - Introduction

- NJOY is a collection of discrete programs that are run in sequence to accomplish a specific goal.
 - Most common usage includes
 - Creation of continuous energy cross section files in “ace” fast format for use with the LANL MCNP(X) continuous energy Monte Carlo programs.
 - Creation of scattering kernel (“ace” thermal) files.
 - Processing covariance data.
 - ◆ Version 2.3 of ERRORJ was merged into NJOY99.259; several of the new updates described below expand this processing capability.
 - Data visualization.
 - ◆ NJOY’s PLOTR/VIEWR modules can be used to create postscript formatted plots.
 - Can display continuous energy cross sections, multigroup cross sections, angular distributions, secondary energy spectra, correlation matrices and uncertainties.

NJOY - Introduction

Code Management

- RSICC or NEA Data Bank distribution includes the basic, uncompiled f77 NJOY99 source code, “src”; the source code for an updating utility program, “upd.f”; various test problem i/o files and various sample makefiles.
- To create an executable
 - Create an executable version of upd.
 - Download the latest available update and appropriate machine dependent patches from <http://t2.lanl.gov/codes/njoy99>.
 - Merge the update file and machine dependent patch files, creating “upn”.
 - With “scr” and “upn” in the same directory, execute upd.
 - ◆ Output will be a series of *.f files for the latest version of NJOY99
 - ◆ Compile and link these files to create the NJOY executable.

NJOY - Introduction

● Code Management (con't)

- Changes to NJOY99 embodied in these patches mean that the sample test problem files accompanying the original distribution are no longer valid.
- Obtain the latest test files from the “t2” web site.
- Small differences are acceptable
 - Test10 which uses random numbers will likely produce different answers (a deficiency that will be rectified in NJOY2008) as a function of User platform.

NJOY - Introduction

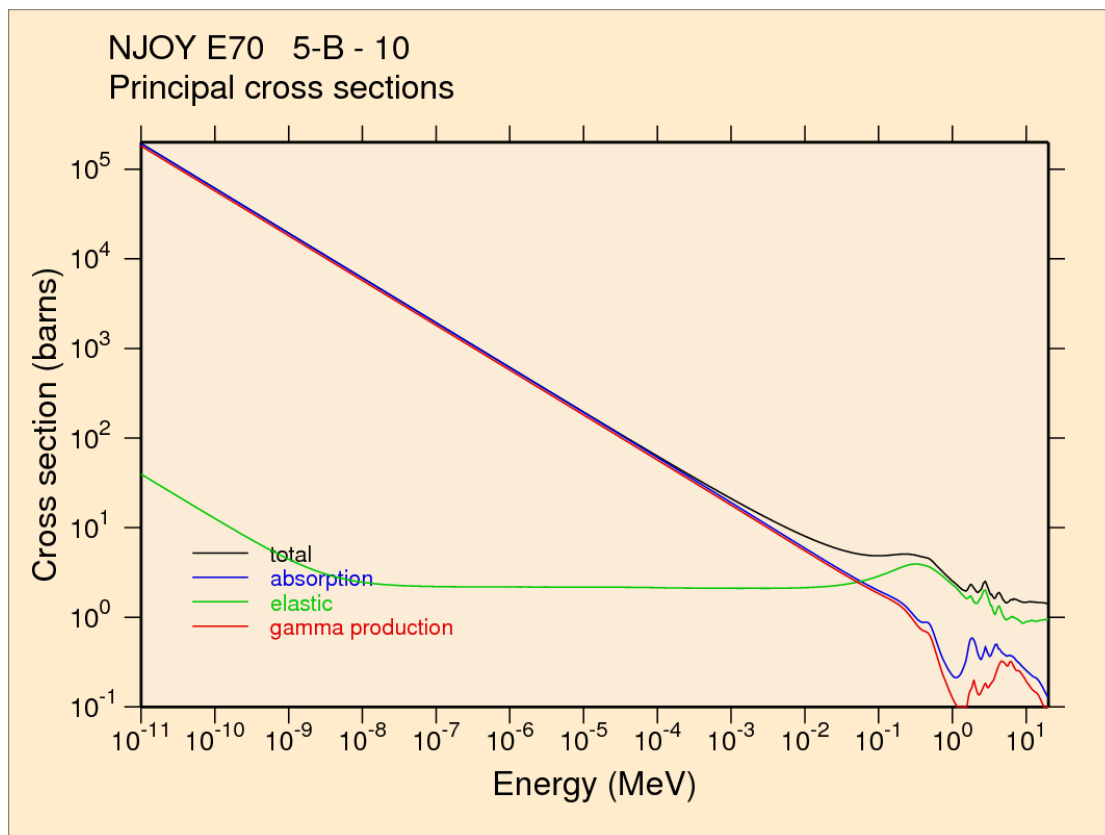
- NJOY interprets a combination of User input instructions plus an ENDF-formatted evaluated data file.
 - NJOY output files conform closely to basic ENDF-formatting rules.
 - A pointwise cross section file output from a given NJOY module is termed a “pendf” file, and is suitable for input to the next NJOY module in the User processing sequence.
 - A groupwise cross section file output by NJOY’s GROUPR module is termed a “gendf” file. While not a formal endf-formatted file, subsequent NJOY modules that further process groupwise data can read this file.
 - ERRORJ’s output file contains a combination of groupwise and covariance matrices that can be read by NJOY’s COVR module which generates correlation matrix, cross section and cross section uncertainty plots.

NJOY – Create Fast ACE Files

Creation of fast ACE files:

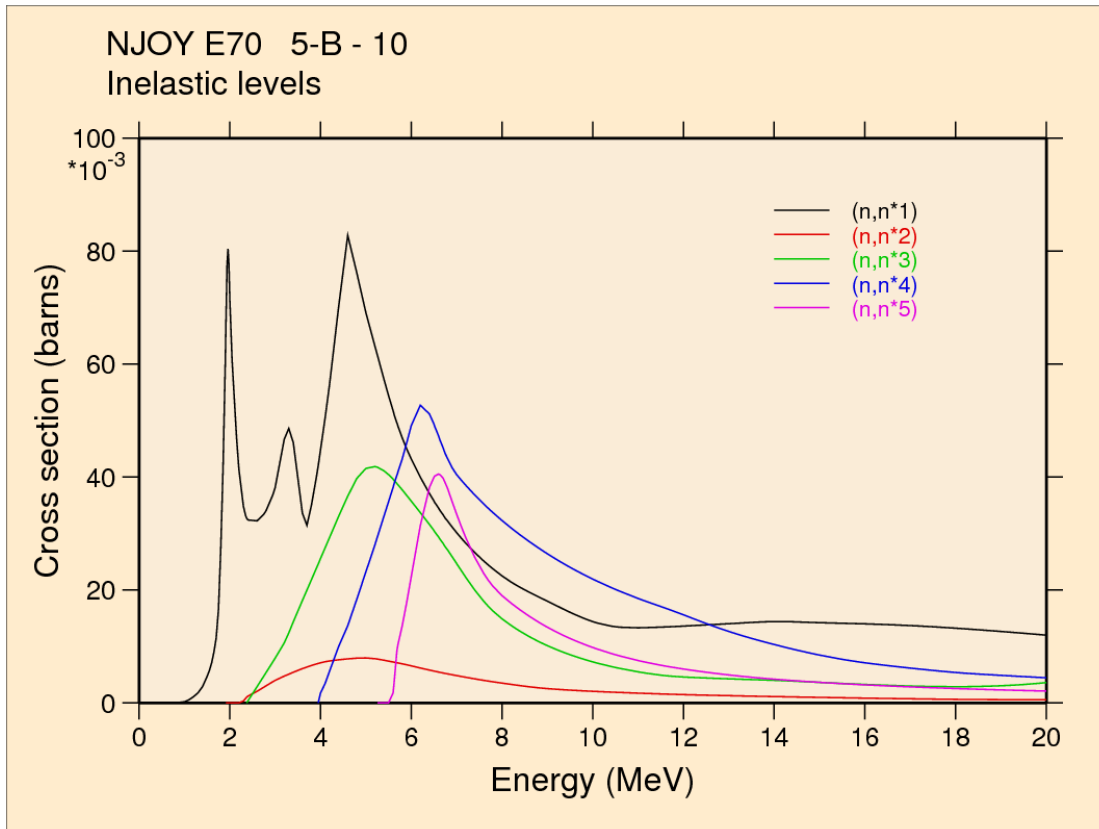
- reconr: expand file2/file3 data to create linearly interpolable continuous energy cross sections.
- broadr: doppler broaden reconr (or previous broadr) output to the desired temperature.
- unresr (optional): calculate unresolved resonance cross sections.
- heatr (optional): calculate energy deposition and damage “cross sections”.
- purr: calculate unresolved resonance probability tables.
- gaspr (optional): calculate gas (^1h , ^2h , ^3h , ^3he and ^4he) production cross section.
- acer: recast output from previous NJOY modules into MCNP fast “ace” format.

NJOY – Fast ACE Plots



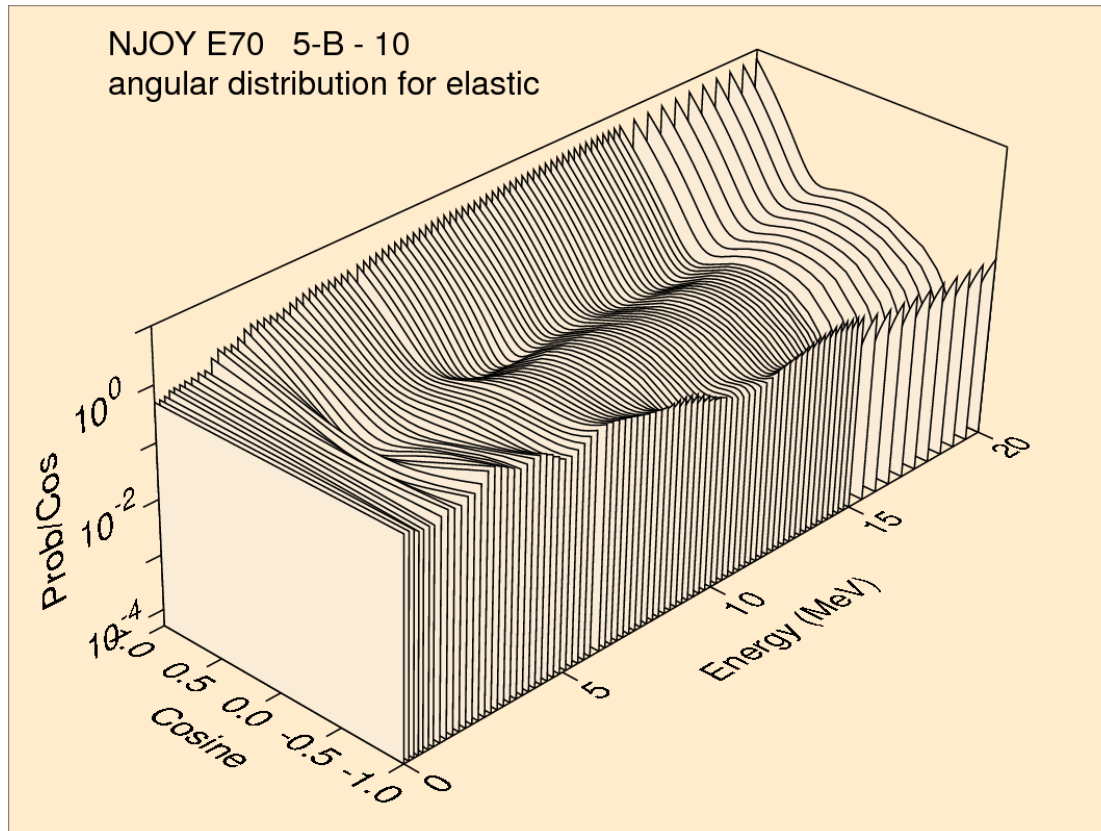
- Doppler broadened continuous energy, linearly interpolable cross sections.

NJOY – Fast ACE Plots



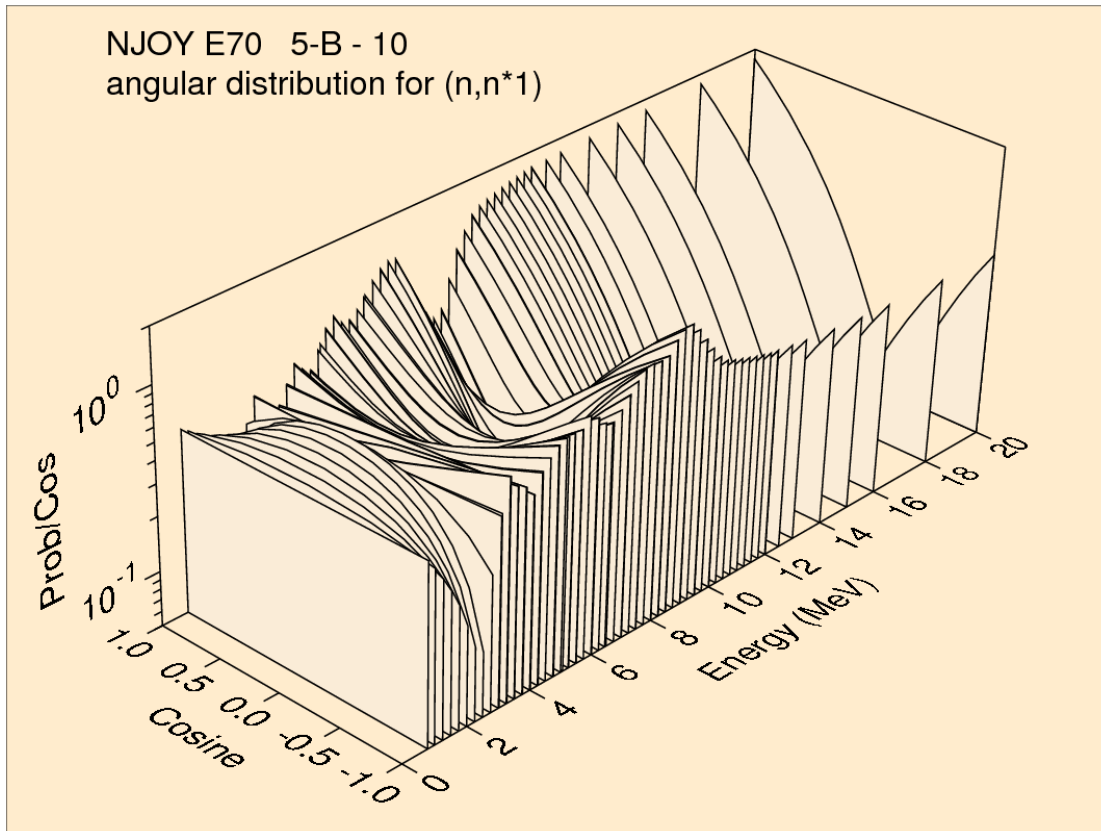
- Example of inelastic cross section plotting.

NJOY – Fast ACE Plots



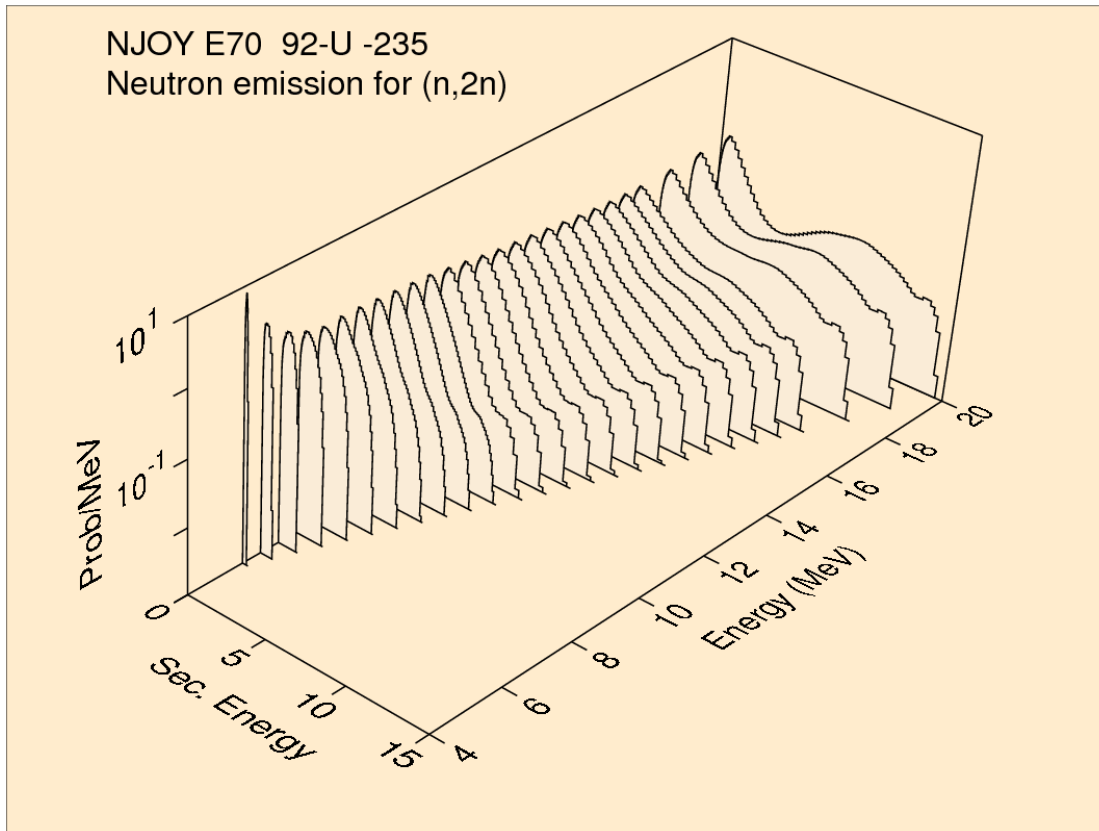
- MF4, MT2 (elastic scattering) angular distributions.

NJOY – Fast ACE Plots



- First inelastic level angular distributions – clearly not isotropic which may be an approximation in older codes.

NJOY – Fast ACE Plots



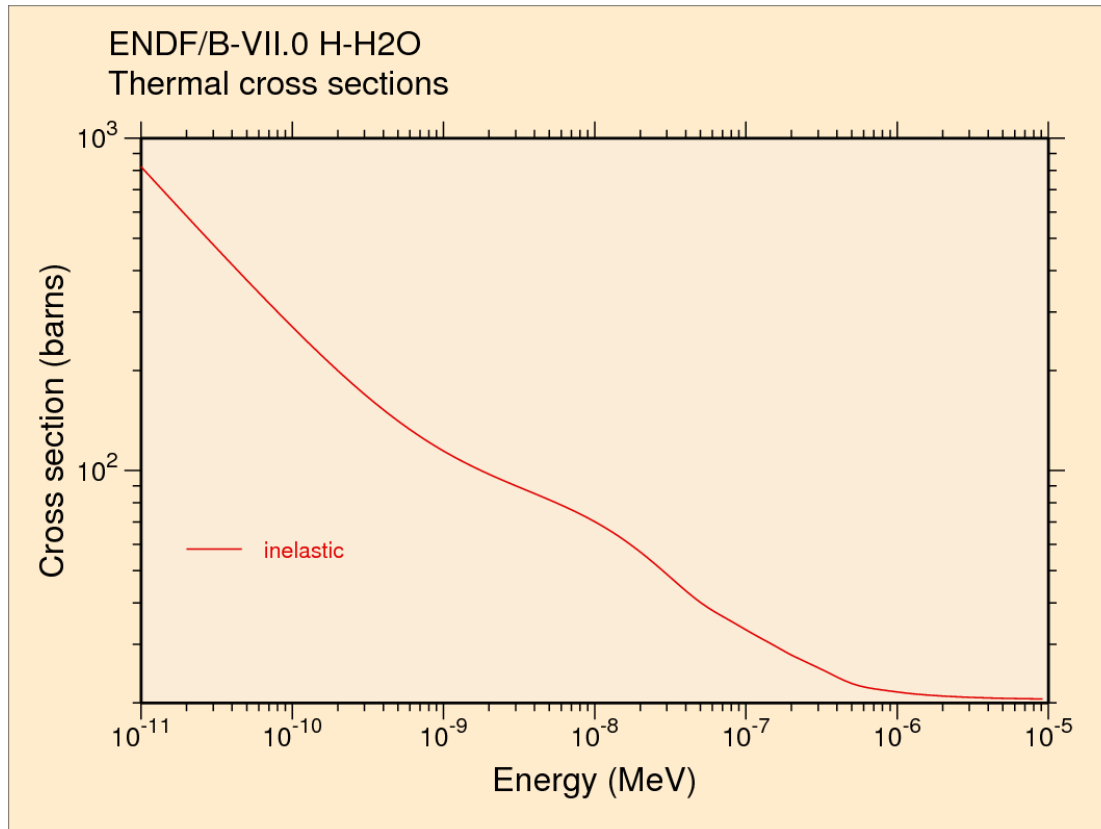
- Secondary neutron emission spectra.

NJOY – Create Thermal ACE Files

● Creation of thermal ACE files

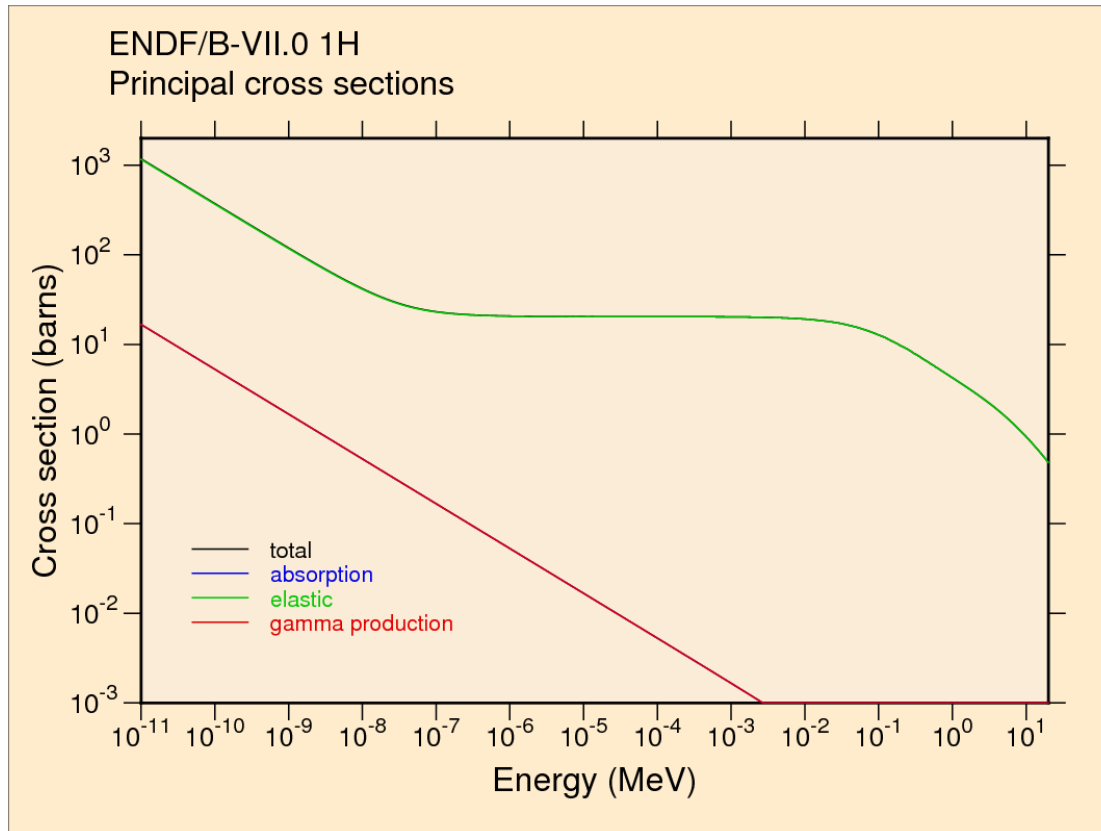
- leapr (optional): use this module to create mf7 thermal scattering kernel data, if not available from a previously generated endf-formatted source.
- thermr: use this module to process leapr output or an endf-formatted thermal kernel input tape.
- acer: convert thermr output to MCNP thermal ace format.

NJOY – Thermal ACE Plots



- Hydrogen bound in water, inelastic scattering.

NJOY – Fast ACE Plots



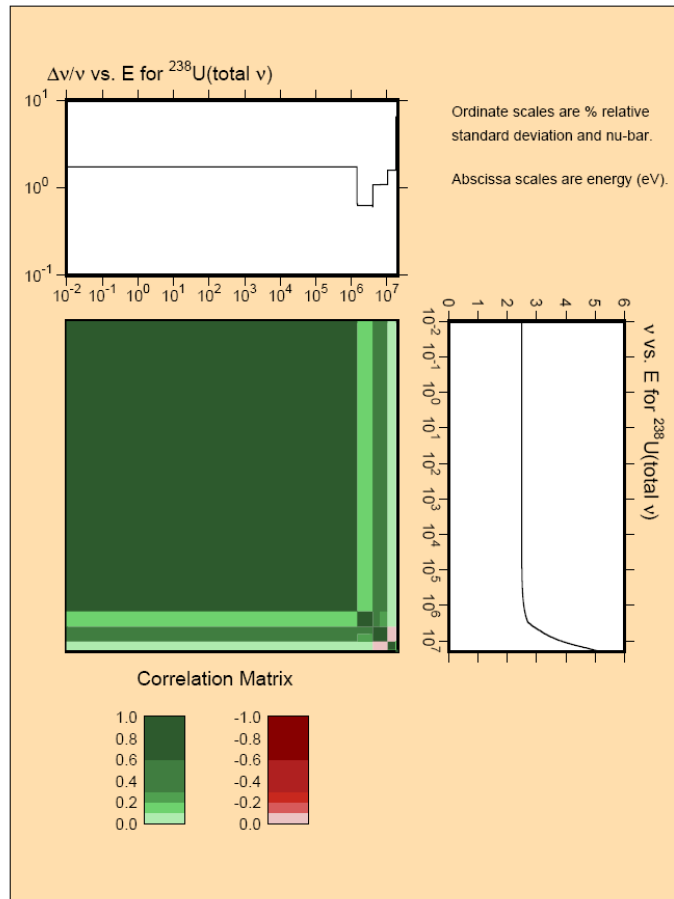
- Free-gas hydrogen
- Note difference in elastic scattering at low energy.

NJOY – Covariance Processing

• Covariance Processing.

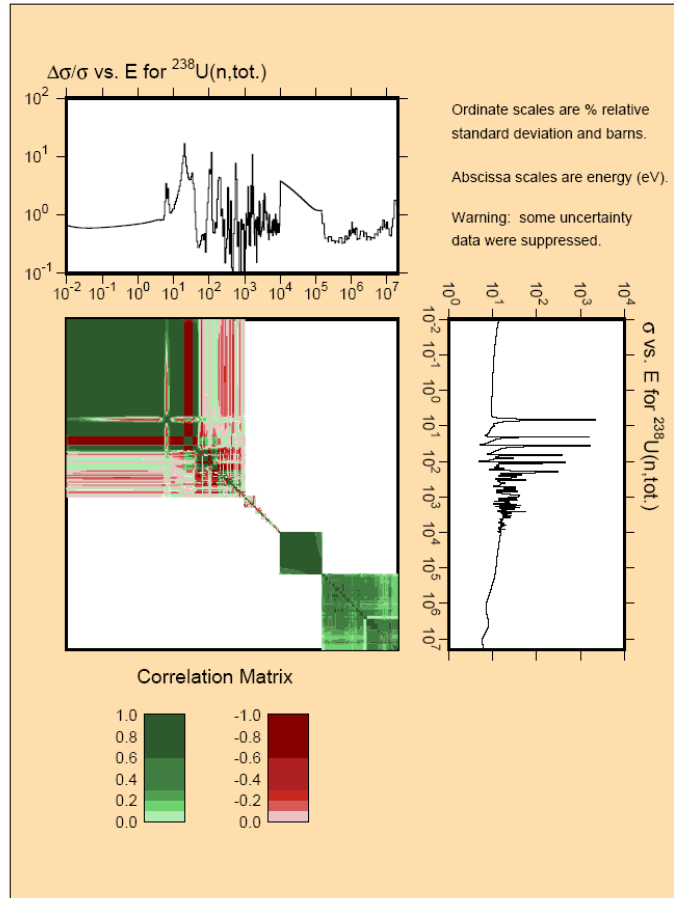
- reconr: expand file2/file3 data to create linearly interpolable continuous energy cross sections.
- broadr: doppler broaden reconr (or previous broadr) output to the desired temperature.
- unresr: calculate unresolved resonance cross sections.
- groupr: calculate group averaged cross sections, angular distributions and emission spectra.
- errorj: process mf31, mf32, mf33, mf34 and mf35 covariance data.
- covr: create plot file for mf31 (nu), mf33 (cross sections), mf34 (mu-bar) or mf35 (spectra), their uncertainties and correlation matrices;
- viewr: convert covr plot file to postscript format.

Covariance Plots – MF31



- New plotting features
 - Uncertainty in data on one frame.
 - Data on the second frame.
 - Use log-log scale for the ordinate when min-to-max ratio is large (currently 10x).
 - Additional color scale so virtually all correlation matrix elements are displayed.
- These data are from JENDL-3.3 ^{238}U .

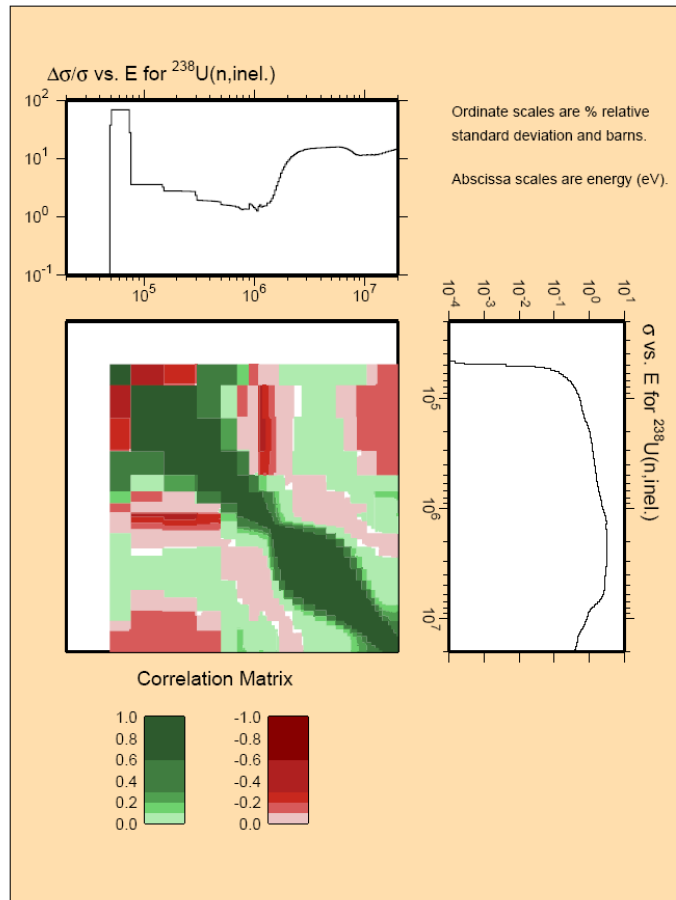
Covariance Plots – MF33



New plot feature

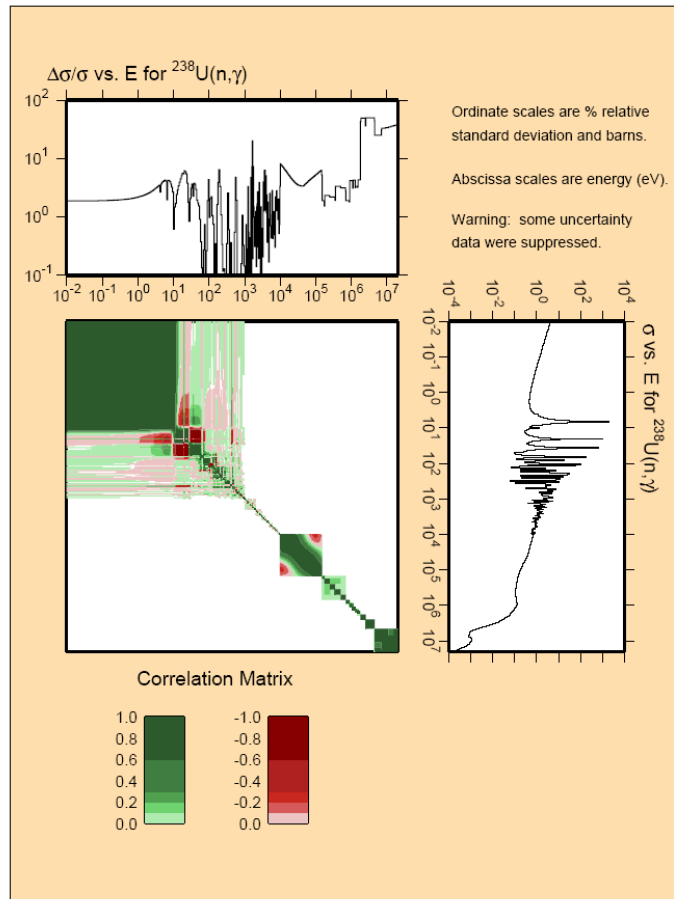
- Warn user when uncertainty data are truncated to fit within the fixed ordinate axis limits.
- Unexpected discontinuities, especially in a derived cross section uncertainty, may indicate a deficiency in the underlying covariance data.

Covariance Plots – MF33



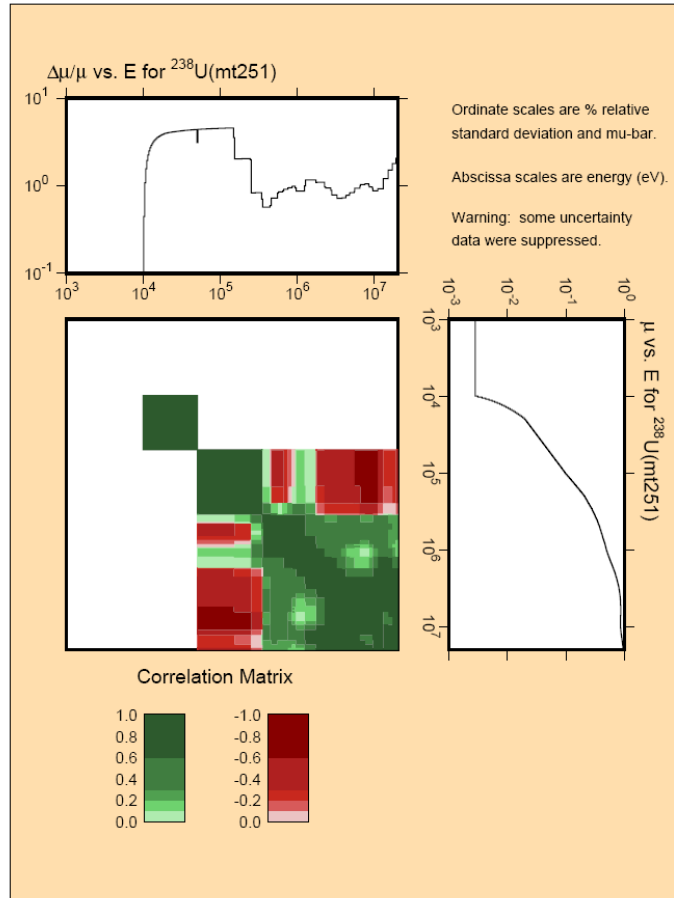
- Axis limits are adjusted to minimize plotting of “zero” data.

Covariance Plots – MF33



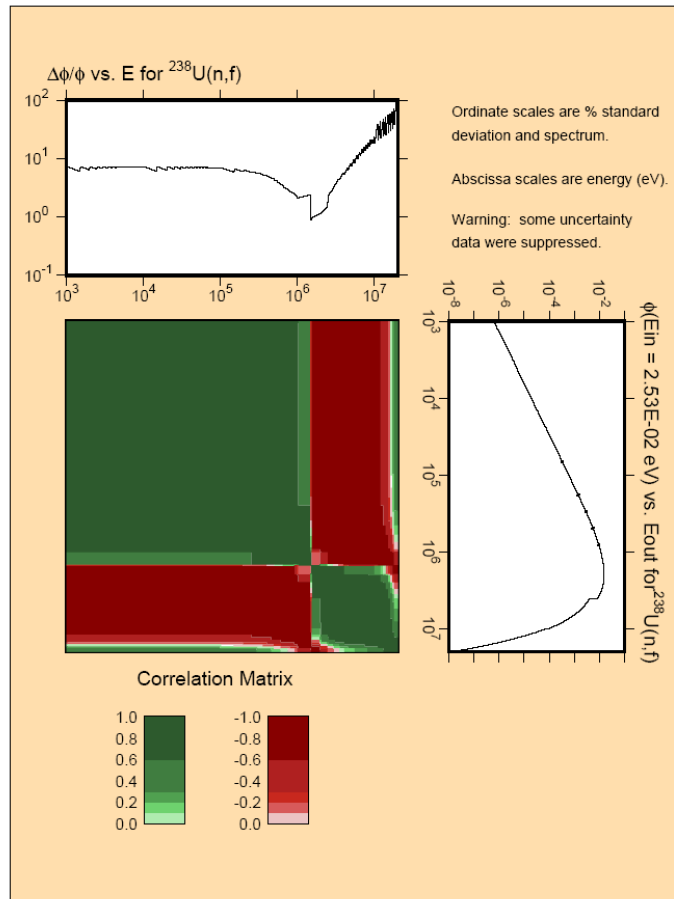
- Again, some features seem unphysical.

Covariance Plots – MF34



- Plotting of mu-bar uncertainty (mt251) is new in NJOY99.279.
- This plot is a 618-group calculation for JENDL-3.3 ^{238}U .

Covariance Plots – MF35



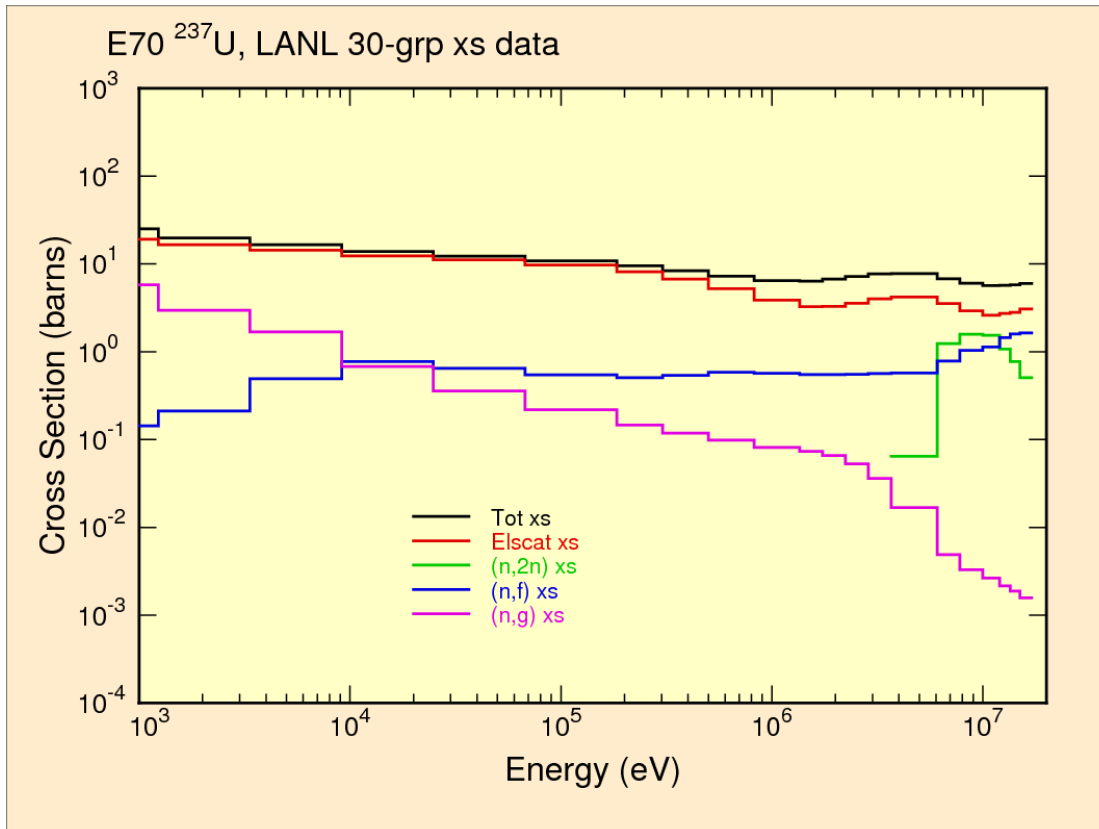
- Plotting of fission spectrum uncertainty (mf5, mt18) is new in NJOY99.279.
- This plot is a 618-group calculation for JENDL-3.3 ^{238}U .

NJOY – Visualization

• Visualization

- NJOY produces a predefined suite of plots, on user option, from the groupr, acer and covr modules.
- User's can also create plots using the plotr and viewr modules.
 - Example follows.

NJOY – PLOTR/VIEWR



- User input to PLOTR to set axis limits, specific MT's, plot title, curve legend, individual curve colors and individual curve line texture.
- This plot generated from GROUPR output.

NJOY2008

- All NJOY99 coding now converted to Fortran 90/95.
 - ➔ No more machine-dependent updates!
 - ➔ Can use Fortran 90/95 intrinsic functions to define these variables.
 - ➔ No more “set sw” to get real*8 precision – now use “kind” definition.
- Historical test problems reproduce NJOY99 results.
 - ➔ New coding includes a “physics” module with various constants collected in one location for easy upgrade.
- A new User manual will accompany the new code.
 - ➔ No more references to NJOY91!

NJOY – Future Developments

- Future Developments (think about this for Friday's NJOY User Group Meeting)
 - Continuing evolution of Covariance formats
 - Scattering radius uncertainty (Rochman/Chiba & revised ERRORJ).
 - An NJOY/CINDER module?
 - A new version of CINDER90 is near release and will contain a room temperature, 63-group, ENDF/B-VII.0 based cross section library.
 - ◆ May also contain JEFF-3.1 and JENDL-3.3 based libraries.
 - Is there User demand to make their own CINDER90 library?
 - Calculate elastic scattering angular distributions from resolved resonance parameters.
 - This capability exists but is not yet tested nor formally implemented in NJOY2008 for LRF=7 (Limited Reich-Moore) evaluations.
 - ◆ Recent data testing of selected ICSBEP benchmarks indicates a large sensitivity in calculated eigenvalue for systems with large axial reflectors as a function of elastic scattering angular distributions.

NJOY – Future Developments

• Future Developments (con't)

- Additional training & web page upgrades.
 - Half-day tutorials at recent technical society meetings have been well attended; may next occur during the ANS general meeting in Atlanta.
 - On-line training was partially implemented for NJOY97 and remains relevant, but is incomplete.
- When should NJOY recognize a deficiency in the basic input file and automatically make corrections?
 - int=2 → int=22 for interpolation of emission spectra.
 - ???
- ???

• Funding for future developments?