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Educational, Scientific and
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International Atomic Energy Agency

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Evaluated data formats and data evaluation with EMPIRE

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Nuclear Data Evaluation, Processing and Applications

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Scope

- Types of nuclear data
- Nuclear reaction data evaluation
- ENDF-6 format
- Data file verification
- Data validation
- Processing for applications

Objectives

- Distinguish different data types and understand the transformations
- Understand the basic principles of data evaluation
- Understand data formatting, verification and validation
- Get acquainted with codes and methods of data processing for applications

Nuclear reaction data types

- Integral (observables in integral measurements)
- Microscopic
  - Differential in incident particle energy
  - Differential in outgoing particle angle or energy (spectra)
  - Double differential in energy and angle
- Processed (result of data reduction)

Nuclear reaction data types

- Microscopic
  - Basic (measured or calculated)
  - Evaluated
- Processed
  - Change of data representation
  - Reformatting
  - Group averaging (preparation of multigroup constants) $\Rightarrow$ **Data Reduction**

What do engineers need?

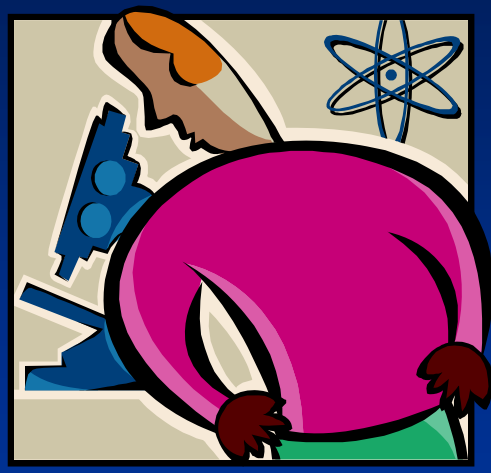
I need cross sections …

$$-\nabla D_{(1)}\nabla\phi_{(1)} + \Sigma_{a(1)}\phi_{(1)} = \frac{1}{k}\left[\sum_{g}\nu_{(g)}\Sigma_{f(g)}\phi_{(g)}\right] + \Sigma_{(2\to1)}\phi_{(2)}$$

$$-\nabla D_{(2)}\nabla\phi_{(2)} + \Sigma_{a(2)}\phi_{(2)} = \Sigma_{(1\to2)}\phi_{(1)}$$

What orthodox theoreticians provide?

Here you are …
It is all described in
my article in the journal !

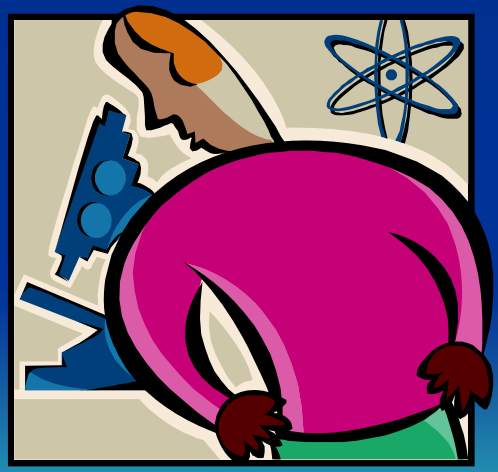


$$\sigma_a(U,J,\pi)=\frac{\pi}{k^2}\frac{(2J+1)}{(2I+1)(2i+1)}\sum_{S=|I-i|}^{I+i}\sum_{l=|J-S|}^{J+S} f(l,\pi)T_l^a(\varepsilon)$$

Dialogue?

What do I do with that?
My codes cannot read journals!

Do what you want!
It's not my job…



Nice guy/girl comes along…

We now have a code
that turns theory
into numbers …

We can compare measured
and calculated data …

… plot pictures …

Are we there yet?

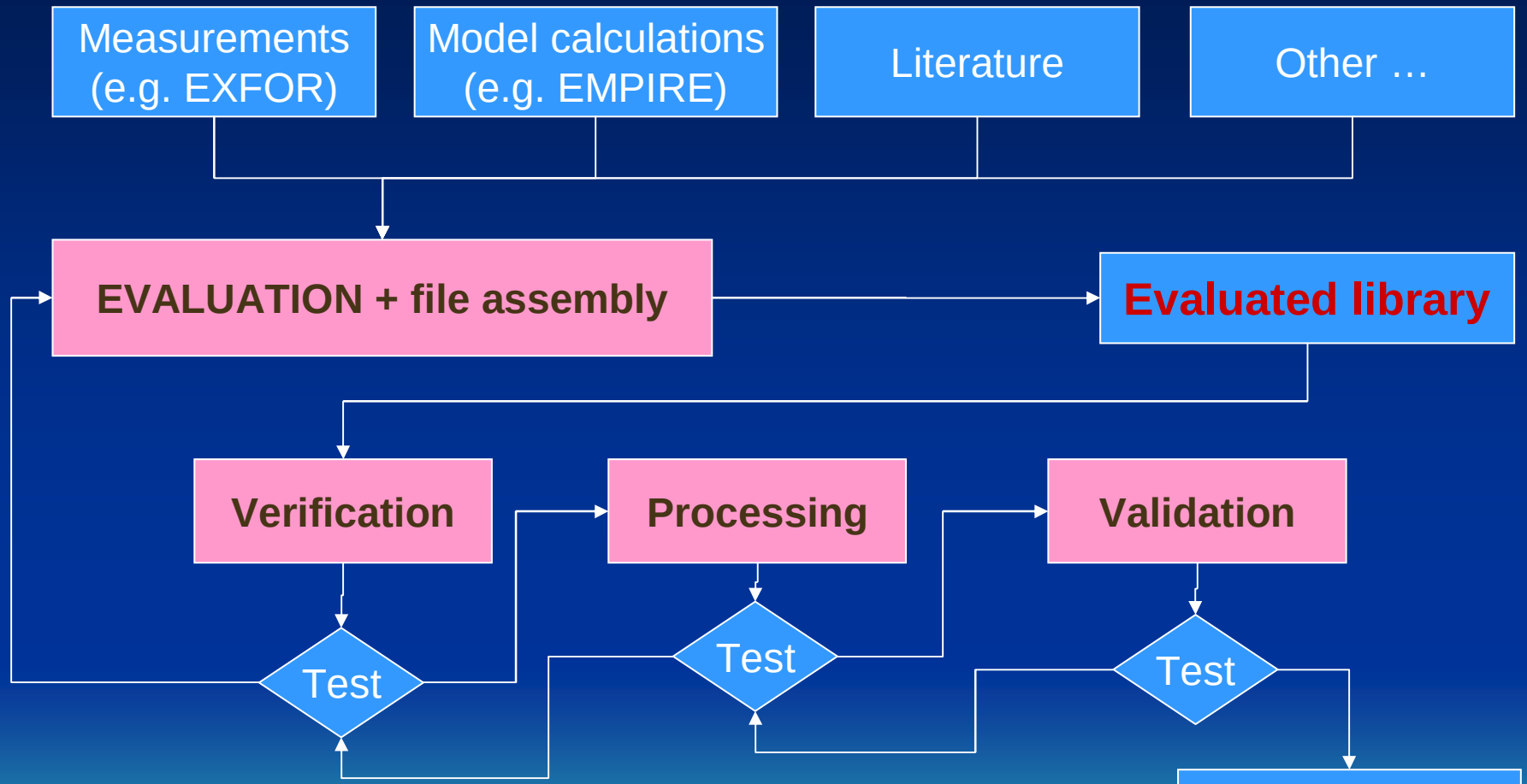
Nice numbers …

Lots of numbers !

Too many numbers !!!

Besides: which one is right ?

What needs to be done?

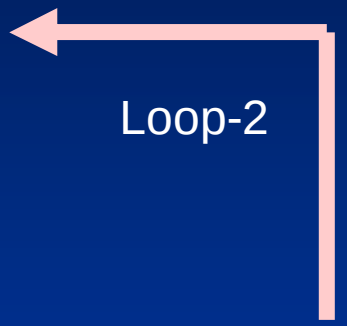


What needs to be done:

- Data evaluation → computer-readable format
- Data reduction (processing)
  - Averaging by energy (deterministic transport) → group-averaged cross sections
  - Reformatting (Monte Carlo transport)
  - Homogenisation and condensation → macroscopic cross sections that engineers need
- Whole-core calculation with thermo-hydraulic feedbacks …

Nuclear reaction data evaluation

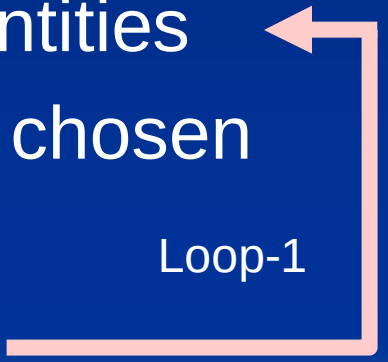
- Evaluation and formatting
- Complete file assembly
- Data file verification
- Processing for applications
- Benchmarking (feedback loop to evaluation)
- Final validation

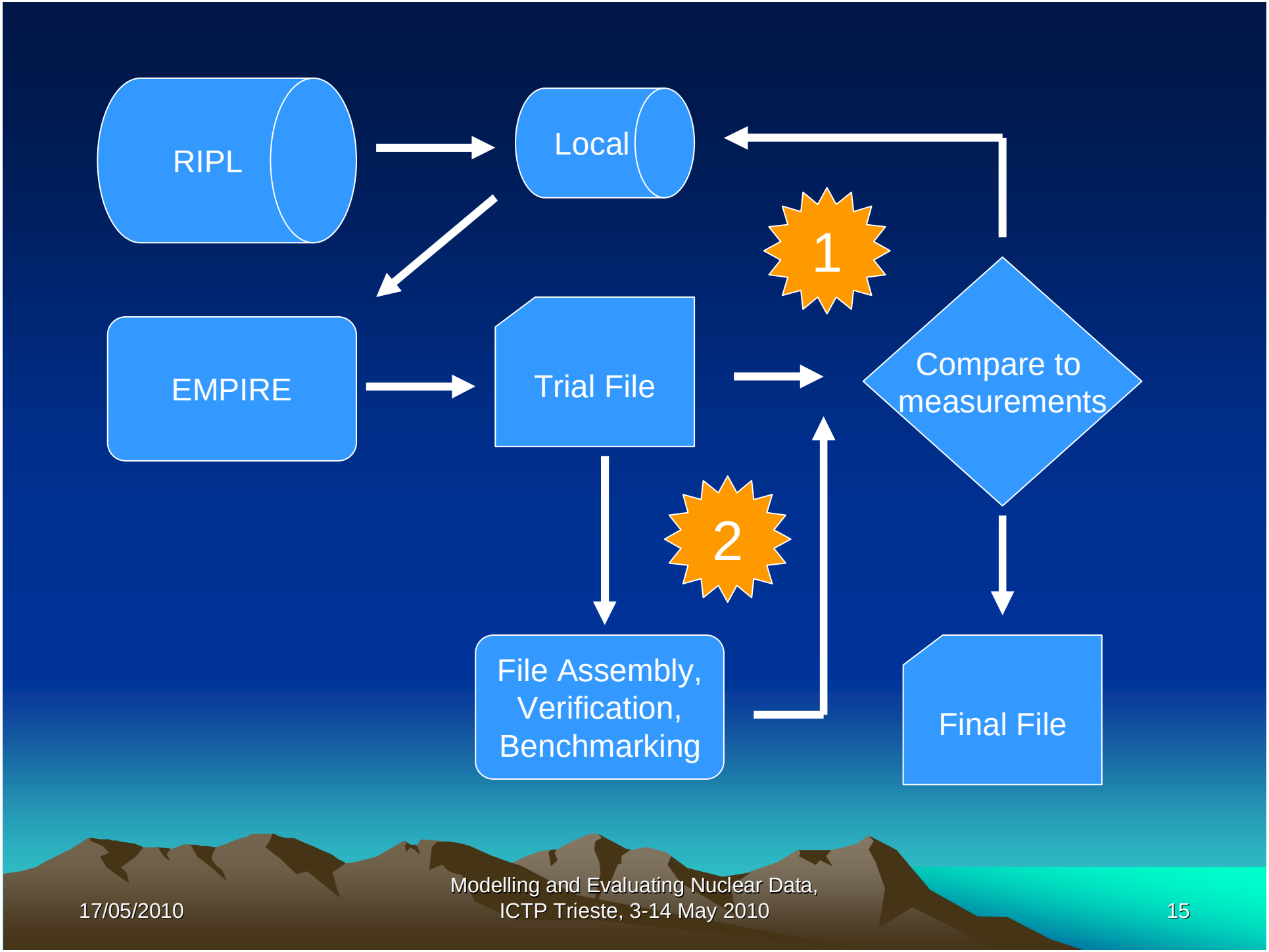


Now we know at least what numbers are (probably) right !

Evaluation – fast energy range

- Use state-of-the-art nuclear model code (EMPIRE)
- Choose adequate model options
- Determine best input parameters (RIPL)
- Calculate cross sections and other quantities
- Compare calculated values to carefully chosen measured data
- Fine-tune the input model parameters
- From model parameter uncertainties generate covariance matrix prior




RIPL
Local
1
EMPIRE
Trial File
Compare to measurements
2
File Assembly, Verification, Benchmarking
Final File

Covariances – fast energy range

- Prior by random sampling of model parameters within their uncertainties
- Introduce measured data (microscopic cross sections and other quantities) to constrain the uncertainties (e.g. GANDR)
- Covariances must be consistent with the evaluated cross section data !

Evaluation – resonance range

- Theoretical predictions are not possible
- Resonance parameters must be obtained from fitting experimental data
- Modern resonance fitting codes produce “best fit” parameters as well as their covariances (e.g. SAMMY, REFIT, etc.)
- Storage of results in ENDF-6 format

ENDF-6 format

- Reasonable compromise between what:
  - Experimentalists can measure
  - Theoreticians can model
  - Engineers can use
- Well documented
  - Precise definitions, >300 pages manual
- Adopted by all national projects
  - USA, EU, Japan, Russia, China …
- Supported by processing codes !

ENDF-6 format (Cont.)

What's in the name?

- Evaluated Nuclear Data File (ENDF)
- "/B" full library from U.S.A. (as opposed to partial evaluations denoted "/A")
- Roman numerals denote library version (e.g. ENDF/B-VII)
- Several releases (updates) may exist (e.g. Rel.1)
- Format designation without "/B" and with arabic numerals for version designation.

ENDF/B-VII Rel.0 – Library from U.S.A.

ENDF-6 Format (maintained by BNL)

Data formatting in ENDF-6

- MAT library sorted by material number
- MF different types of data
- MT reaction types

Data formatting ENDF-6

MF different types of data

1	General information, nu-bar, decay data, etc.
2	Resonance parameters
3	Cross sections
4	Angular distributions
5	Emission spectra
6	Double differential cross-sections
32	Resonance parameter covariances
33	Cross section covariances
34	Angular distribution covariances
35	Emission spectra covariances, etc.

Data formatting ENDF-6

MT different reaction types

1	Total
2	Elastic
16	(n,2n)
18	Fission
51-91	Discrete inelastic and continuum
102	Radiative capture
600-649	Discrete level proton emission
800-849	Discrete level alpha emission

Etc.

```
IRDF-ext                                                        777 0  0     0
 5.312700+4 1.258140+2          2          0         41          15325 1451     1
 0.000000+0 0.000000+0          0          0          0          65325 1451     2
 1.000000+0 3.200000+7          0          0         10          25325 1451     3
 0.000000+0 0.000000+0          1          0        122          35325 1451     4
 53-I -127 FEI         EVAL-Jul07 K.I.Zolotarev                   5325 1451     5
                       DIST-Sep07                                 5325 1451     6
----BROND-2            MATERIAL 5325                              5325 1451     7
-----INCIDENT NEUTRON DATA                                        5325 1451     8
------ENDF-6 FORMAT                                              5325 1451     9
**************************************************************** 5325 1451    10
* Extension to the International Reactor Dosimetry Library      * 5325 1451    11
* supported partially by the International Atomic Energy Agency * 5325 1451    12
* through IAEA research contract 13335.                         * 5325 1451    13
.
.
.
 0.000000+0 0.000000+0          0          0          0           05325 0  0     0
 5.312700+4 1.258140+2          0          0          0           05325 3 16     1
-9.143470+6-9.143470+6          0          0          1         1745325 3 16     2
         174           2                                          5325 3 16     3
 9.215700+6 0.000000+0 9.250000+6 1.050030-2 9.450000+6 1.745260-25325 3 16     4
 9.500000+6 2.822020-2 9.550000+6 4.175640-2 9.600000+6 5.772310-25325 3 16     5
 9.650000+6 7.581830-2 9.700000+6 9.577150-2 9.750000+6 1.173390-15325 3 16     6
 9.800000+6 1.403000-1 9.850000+6 1.644570-1 9.900000+6 1.896270-15325 3 16     7
```

Evaluated data file assembly

- Data for the resonance and fast range must be assembled consistently (ENDRES)
  - Resolved resonance range
  - Unresolved resonance range (LSSF flag)
  - Background contribution in MF 3
- Covariance data inserted when ready (ENDCOV)
  - Energy range consistency of MF32 with MF2
  - Energy range consistency of MF32 and MF33

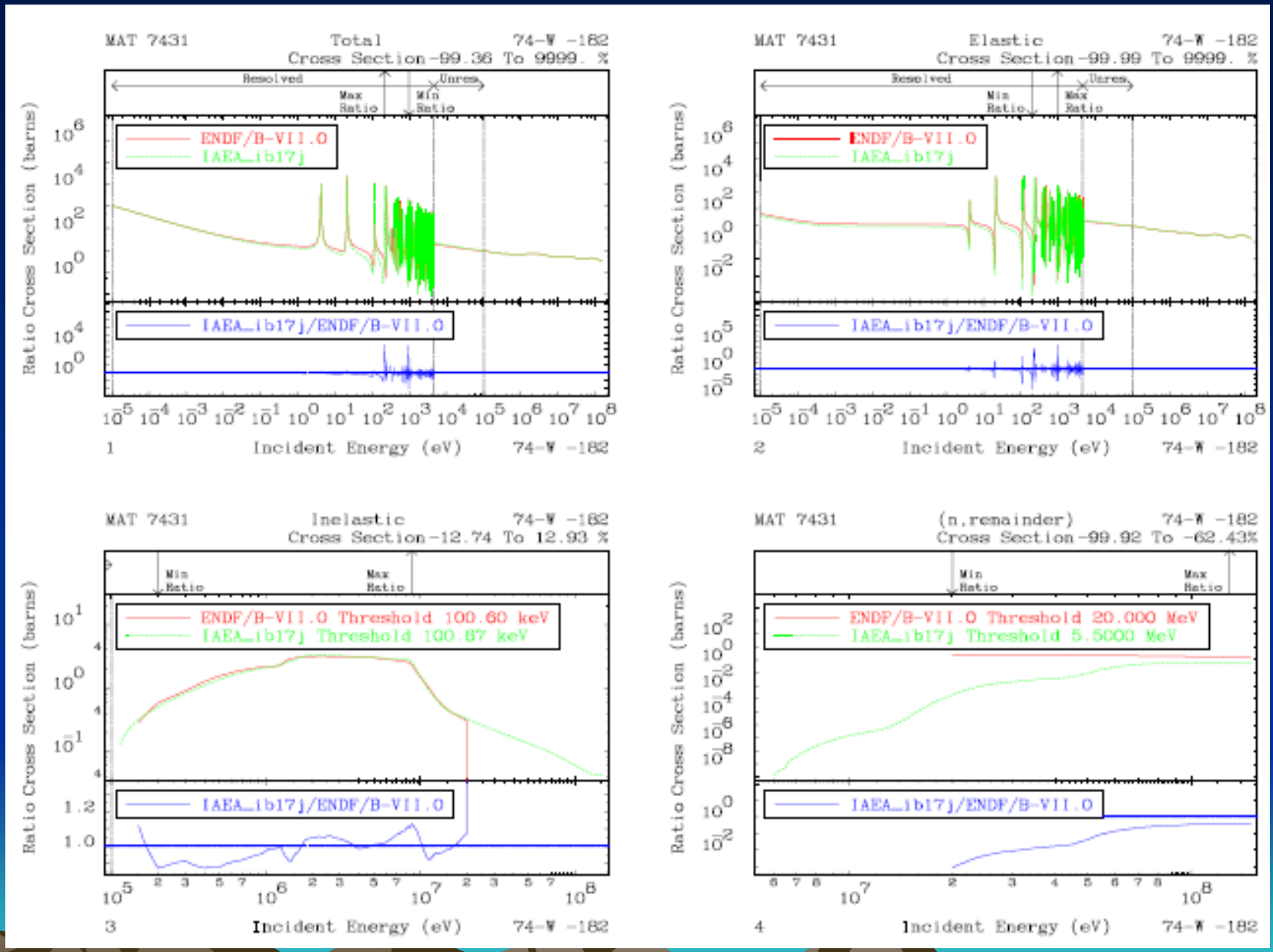
WARNING: Patching into the file covariance data from another evaluation is *dangerous !*

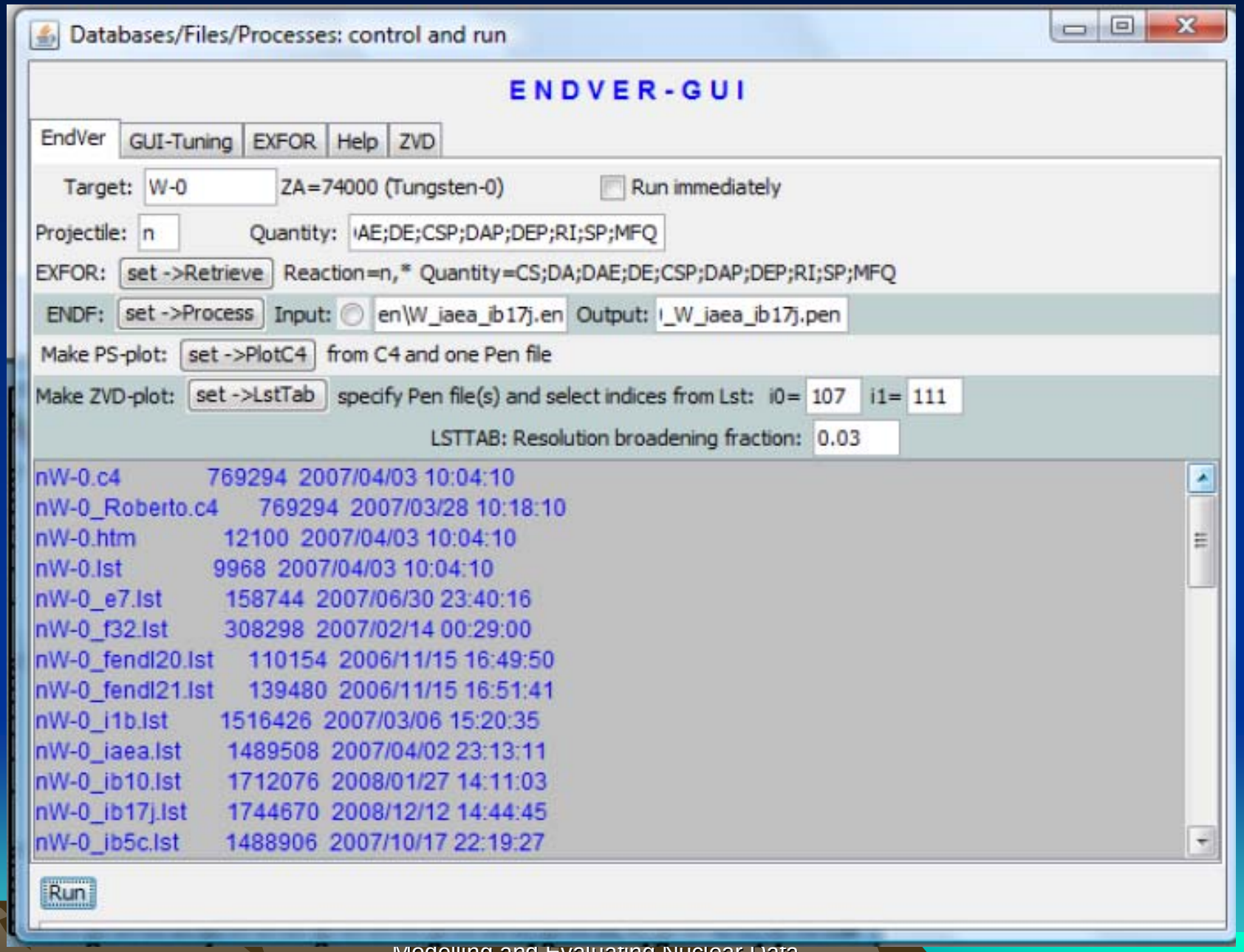
Evaluated file verification

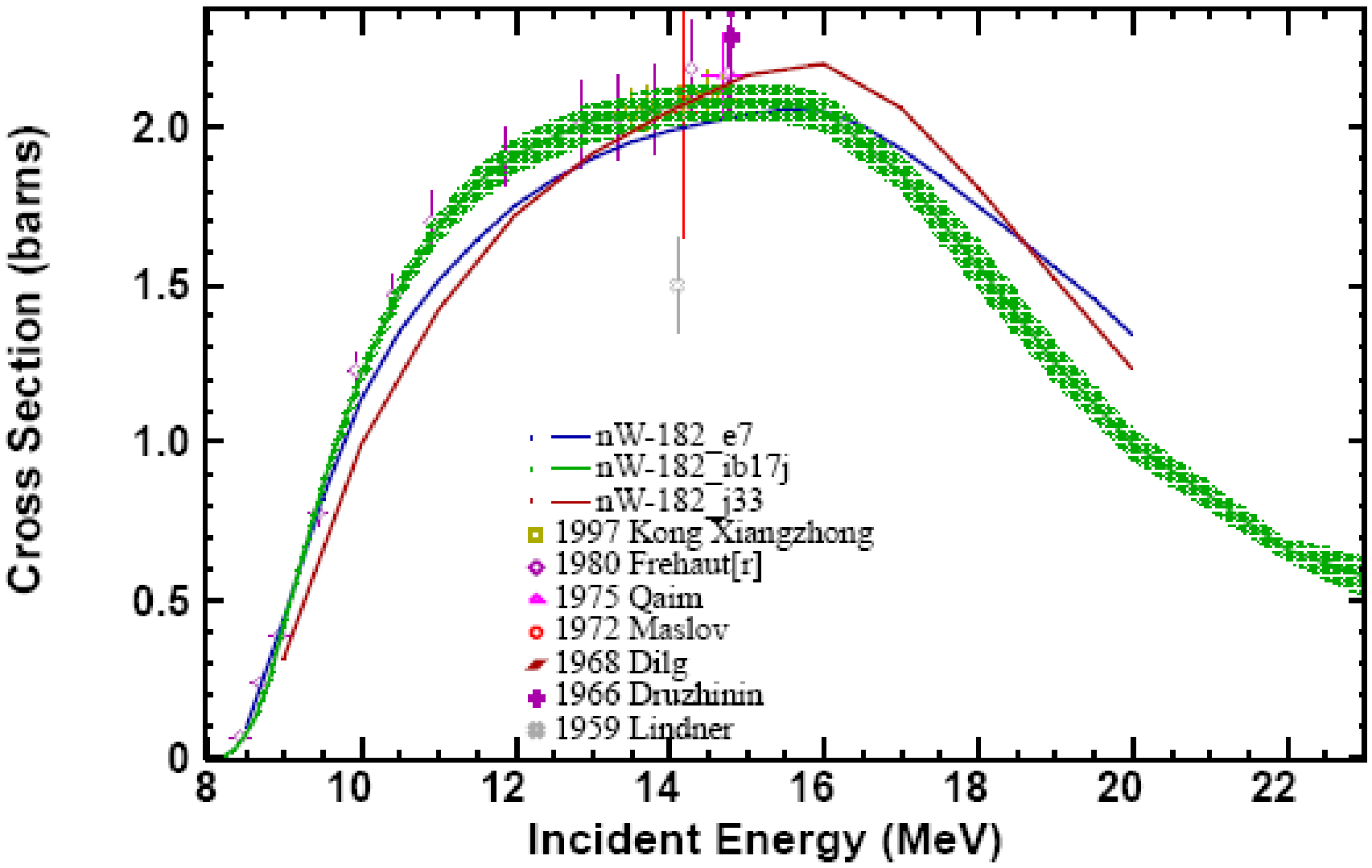
- ENDF Utility codes
  - STANEF: utility to standardise number representation, dictionary, etc.
  - CHECKR: check formal correctness of format
  - FIZCON: check physical consistency of the data
  - PSYCHE: more advanced checking of the file contents

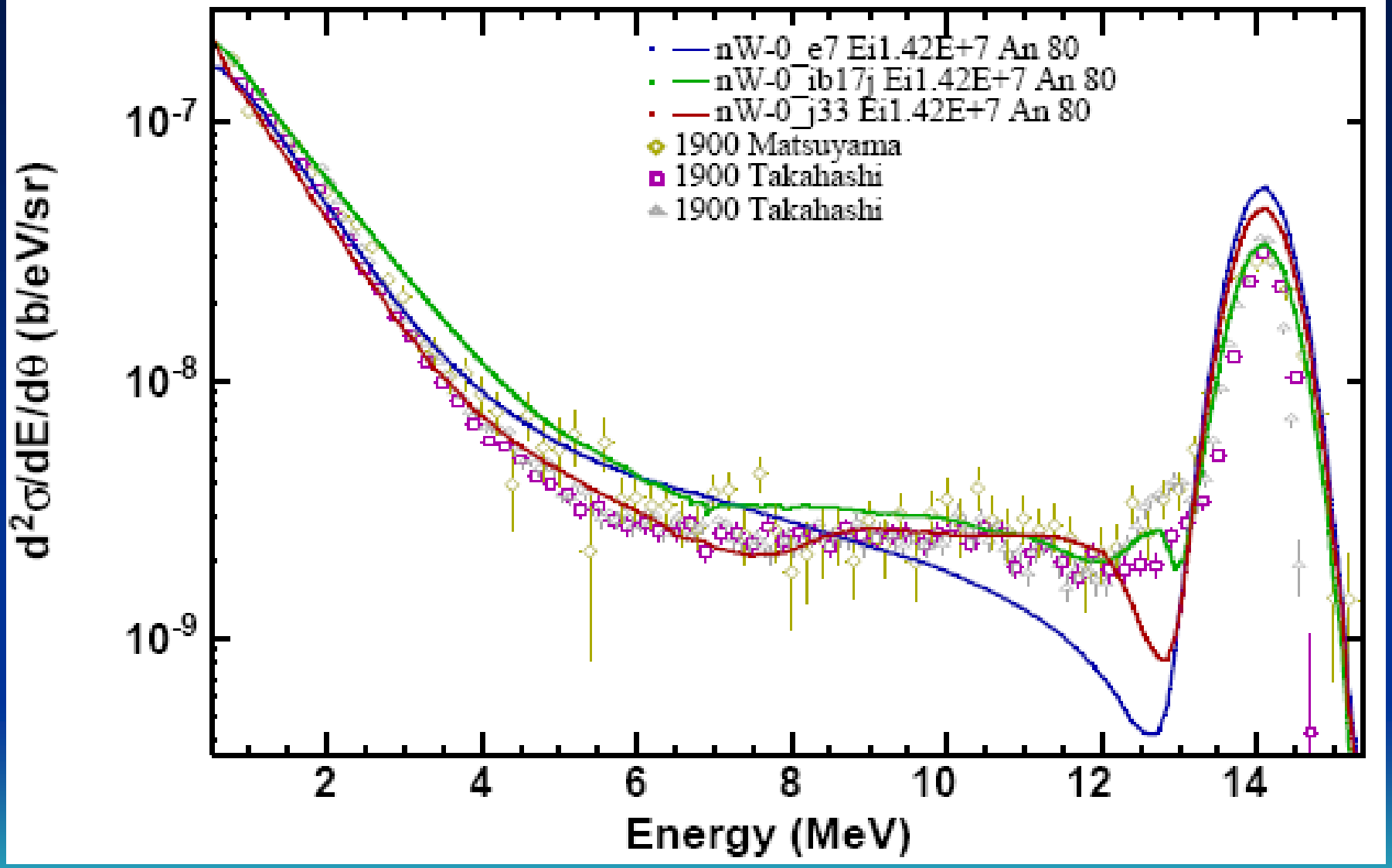
Evaluated file verification (Cont.)

- Pre-Pro ENDF Pre-Processing codes
  - Linearisation, resonance reconstruction, Doppler broadening, etc.
  - First test of data processability.
- ENDVER graphical display package
  - Heavy usage of Pre-Pro codes
  - Comparison with experimental data from EXFOR
  - Reconstruction of elemental data from isotopic
  - Reactions defined by summation
  - Differential and double-differential data


MAT 7431
Total
74-W -182
Cross Section -99.36 To 9999. %
Resolved
Unres
Max Ratio
Min Ratio
ENDF/B-VII.0
IAEA_ib17j
IAEA_ib17j/ENDF/B-VII.0
Ratio Cross Section (barns)
1
Incident Energy (eV)
74-W -182
MAT 7431
Elastic
74-W -182
Cross Section -99.99 To 9999. %
Resolved
Unres
Min Ratio
Max Ratio
ENDF/B-VII.0
IAEA_ib17j
IAEA_ib17j/ENDF/B-VII.0
Ratio Cross Section (barns)
2
Incident Energy (eV)
74-W -182
MAT 7431
Inelastic
74-W -182
Cross Section -12.74 To 12.93 %
Min Ratio
Max Ratio
ENDF/B-VII.0 Threshold 100.60 keV
IAEA_ib17j Threshold 100.67 keV
IAEA_ib17j/ENDF/B-VII.0
Ratio Cross Section (barns)
3
Incident Energy (eV)
74-W -182
MAT 7431
(n,remainder)
74-W -182
Cross Section -99.92 To -62.43%
Min Ratio
Max Ratio
ENDF/B-VII.0 Threshold 20.000 MeV
IAEA_ib17j Threshold 5.5000 MeV
IAEA_ib17j/ENDF/B-VII.0
Ratio Cross Section (barns)
4
Incident Energy (eV)
74-W -182


Databases/Files/Processes: control and run
ENDVER-GUI
EndVer
GUI-Tuning
EXFOR
Help
ZVD
Target: W-0
ZA=74000 (Tungsten-0)
Run immediately
Projectile: n
Quantity: AE;DE;CSP;DAP;DEP;RI;SP;MFQ
EXFOR: set ->Retrieve
Reaction=n,* Quantity=CS;DA;DAE;DE;CSP;DAP;DEP;RI;SP;MFQ
ENDF: set ->Process
Input: en\W_jaea_ib17j.en
Output: _W_jaea_ib17j.pen
Make PS-plot: set ->PlotC4
from C4 and one Pen file
Make ZVD-plot: set ->LstTab
specify Pen file(s) and select indices from Lst: i0= 107 i1= 111
LSTTAB: Resolution broadening fraction: 0.03
nW-0.c4 769294 2007/04/03 10:04:10
nW-0_Roberto.c4 769294 2007/03/28 10:18:10
nW-0.htm 12100 2007/04/03 10:04:10
nW-0.lst 9968 2007/04/03 10:04:10
nW-0_e7.lst 158744 2007/06/30 23:40:16
nW-0_f32.lst 308298 2007/02/14 00:29:00
nW-0_fendl20.lst 110154 2006/11/15 16:49:50
nW-0_fendl21.lst 139480 2006/11/15 16:51:41
nW-0_i1b.lst 1516426 2007/03/06 15:20:35
nW-0_jaea.lst 1489508 2007/04/02 23:13:11
nW-0_jb10.lst 1712076 2008/01/27 14:11:03
nW-0_jb17j.lst 1744670 2008/12/12 14:44:45
nW-0_jb5c.lst 1488906 2007/10/17 22:19:27
Run


Cross Section (barns)
Incident Energy (MeV)
0
0.5
1.0
1.5
2.0
8
10
12
14
16
18
20
22
nW-182_e7
nW-182_ib17j
nW-182_j33
1997 Kong Xiangzhong
1980 Frehaut[r]
1975 Qaim
1972 Maslov
1968 Dilg
1966 Druzhinin
1959 Lindner


nW-0_e7 Ei1.42E+7 An 80
nW-0_ib17j Ei1.42E+7 An 80
nW-0_j33 Ei1.42E+7 An 80
1900 Matsuyama
1900 Takahashi
1900 Takahashi
d²σ/dEdθ (b/eV/sr)
10⁻⁷
10⁻⁸
10⁻⁹
2
4
6
8
10
12
14
Energy (MeV)

Data processing

- Reformatting and basic operations
  - Linearization
  - Resonance reconstruction
  - Doppler broadening, etc.
- Data reduction
  - Averaging over energy
  - Averaging over space
- Assembly of application libraries

Data Reduction: Group averaging over energy

Reaction Rates

$$\sigma_g \varphi_g = \int_g \sigma(E).\varphi(E)dE$$

Average Cross Sections

$$\varphi_g = \int_g \varphi(E)dE$$

$$\sigma_g = \frac{\int_g \sigma(E)\varphi(E)dE}{\int_g \varphi(E)dE}$$

Scattering Matrices

$$\sigma_{(l)g\to h} = \frac{\int_{-1}^{1} d\mu \int_g dE.\varphi(E) \int_h dE'.\sigma\left(E \to E', \mu\right).P_l\left(\mu\right)}{\int_g \varphi\left(E\right).dE}$$

Data Reduction: Group averaging over space

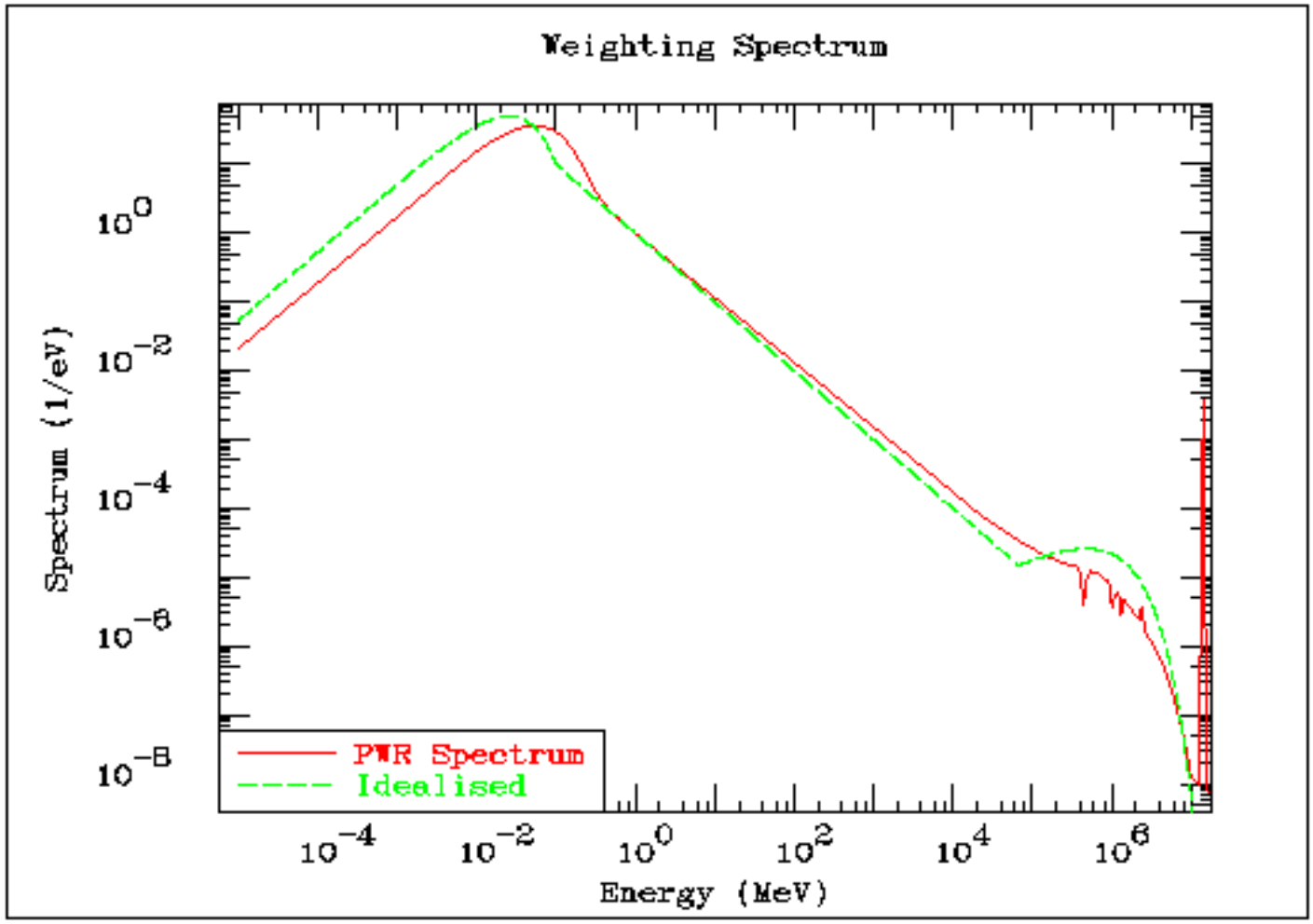
Reaction Rates

$$\left\langle \Sigma_g \right\rangle \left\langle \phi_g \right\rangle = \int_V \Sigma(\vec{r})\phi(\vec{r})dV$$

Average flux and cross sections

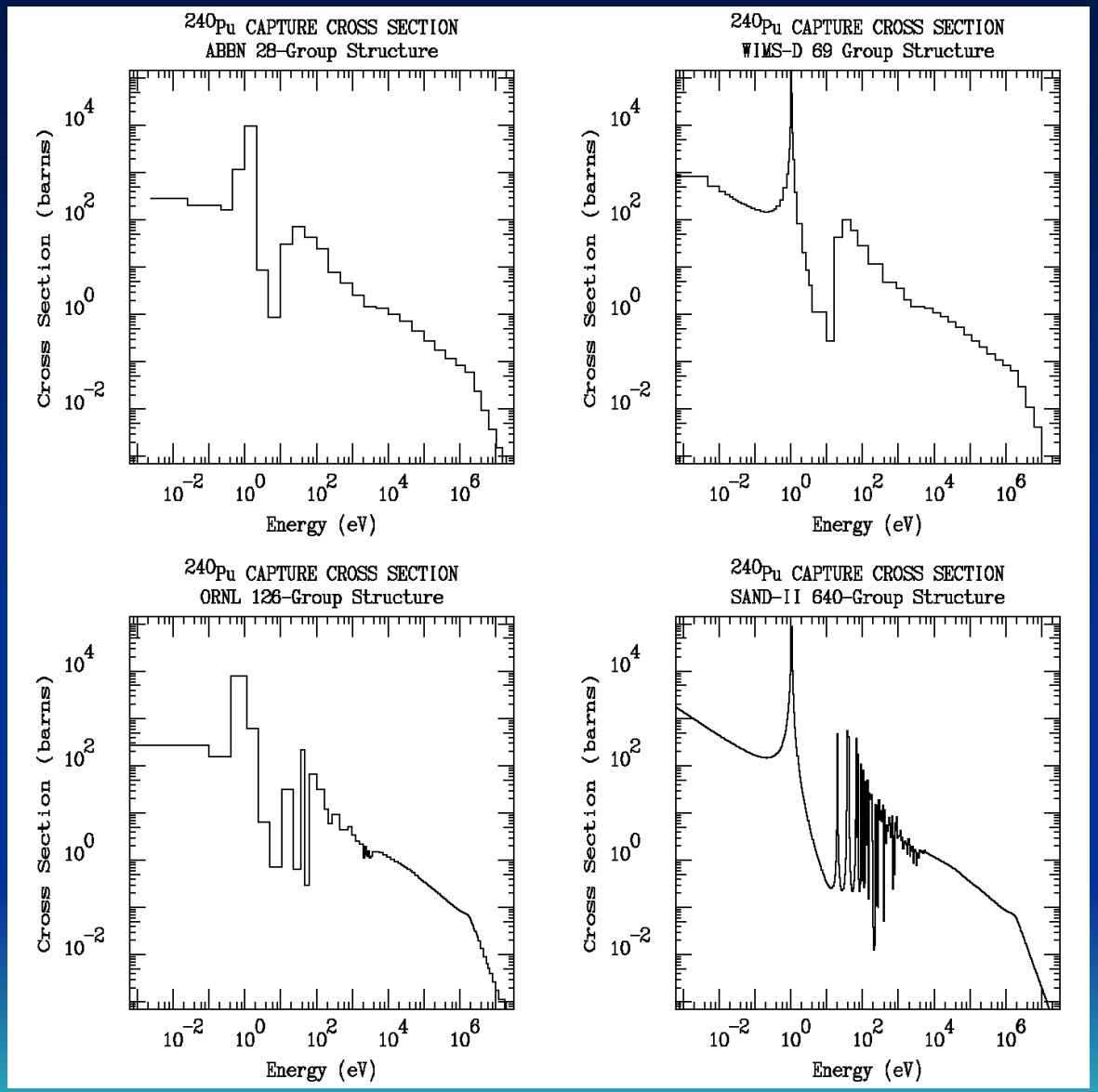
$$\left\langle \phi_g \right\rangle = \int_V \phi(\vec{r})dV$$

$$\left\langle \Sigma_g \right\rangle = \frac{\int_V N\sigma(\vec{r})\phi(\vec{r})dV}{\int_V \phi(\vec{r})dV}$$


Weighting Spectrum
Spectrum (1/eV)
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
PWR Spectrum
Idealised
10^{-4}
10^{-2}
10^{0}
10^{2}
10^{4}
10^{6}
Energy (MeV)

Group averaged data - Definitions

- Fine group data (> about 600 groups)
- Multigroup (20 – 600 groups)
  - Application-dependent (fast reactors, thermal reactors, fusion applications, accelerator shielding, etc.
- Few-group (1-20 groups)
  - Local material properties (macroscopic cross sections, homogenised coarse-mesh spatial grid)


240Pu CAPTURE CROSS SECTION
ABBN 28-Group Structure
240Pu CAPTURE CROSS SECTION
WIMS-D 69 Group Structure
240Pu CAPTURE CROSS SECTION
ORNL 126-Group Structure
240Pu CAPTURE CROSS SECTION
SAND-II 640-Group Structure
Cross Section (barns)
Energy (eV)

Data Processing codes

- Pre-Pro: ENDF Pre-Processing codes perform basic operations on nuclear data
- NJOY is a comprehensive system for generating application libraries, developed at Los Alamos National Laboratory
- AMPX is a comparable system developed at Oak Ridge National Laboratory

Covariances

- Sensitivity vector *S* of the sensitivity of parameters x_i y_j to integral observable R

$$S_i = \frac{x_i \; dR}{R \; dx_i}$$

- Group representation *i*
- Covariance matrix $\mathbf{C}(x_i,y_j)$
- Uncertainty by the sandwich rule

$$dR = S^T \mathbf{C} S$$

Covariances (cont.)

Covariance matrix prior in the fast energy range

- Best-estimate evaluation (model calculation)
- Perturbation by random sampling of the model parameters and tuning factors
- Covariance matrix prior, including correlations between energies and reaction channels

Covariances (cont.)

Covariance matrix of resonance parameters

- Resonance analysis is usually done separately
- Covariances of resonances parameters are obtained during resonance analysis
- Resonance analysis codes usually provide parameters in ENDF-6 format

Covariances (cont.)

Experimental data

- Correlations in experimental data
- Scheme to apply GLSQM or UMCM (e.g. GANDR system)
- Apply adjustments to cross sections
- Insert covariances into ENDF files
- Analysis may include cross-material correlations

Data validation

- Before use, verification of application libraries is needed (processing errors)
- Validation of evaluated data files is implicit in the validation of application libraries
- Validation of application libraries is done by modelling integral benchmarks and comparing calculated and measured integral parameters
- Validity of such libraries is limited to problems, which resemble the benchmark test cases.

Data validation (Cont.)

- Verification: CHECKR, FIZCON, PSYCHE, EMPEND…
- Processing: NJOY (for deterministic and/or Monte Carlo codes) → test application library
- Validation: benchmark databases ICSBEP, IRPhE, SINBAD … → Compare calculations/experiment

Conclusions

- Evaluation steps described
- Covariance data preparation described
- Verification steps defined
- Validation:
  - Processing
  - Benchmark calculations
  - Feedback to evaluation
  - Validity: cases similar to benchmarks