Nuclear Data for Power 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 verification and validation
- Get acquainted with codes and methods of data processing for applications

Nuclear reaction data types

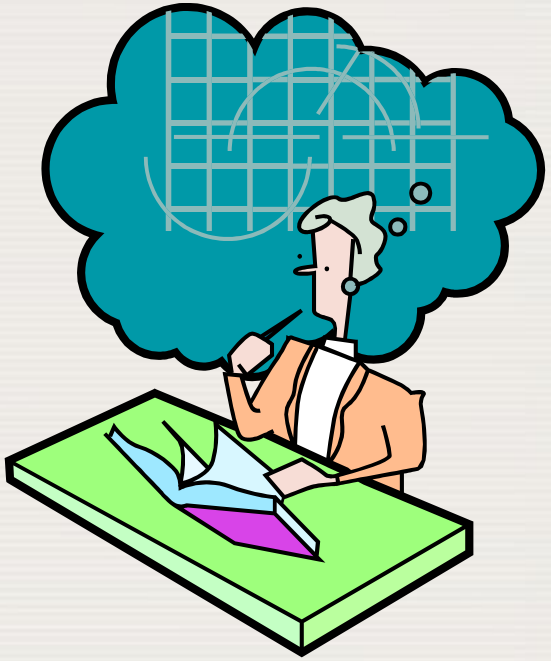
- **Integral** - observables in integral measurements – (e.g. reaction rates, k_{eff})
- **Microscopic** (cross sections)
  - Differential in incident particle energy
  - Differential in outgoing particle angle or energy (spectra)
  - Double differential in energy and angle
- **Processed** (result of data reduction)

Nuclear reaction data types

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

What do engineers need?

I need cross sections …

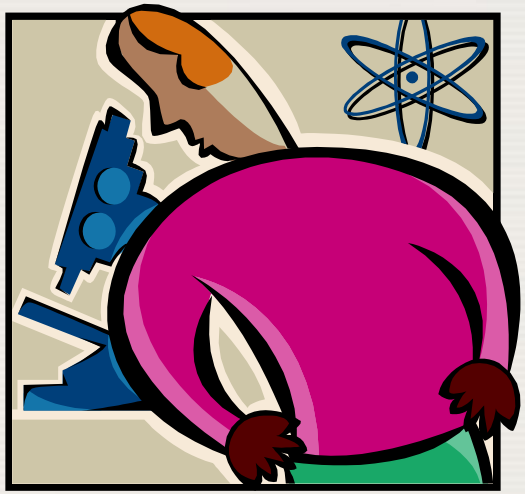


$$-\nabla D_{(1)}\nabla\phi_{(1)} + \Sigma_{a(1)}\phi_{(1)} = \frac{1}{k}\left[\sum_{g}\nu_{(g)}\Sigma_{f(g)}\phi_{(g)}\right] + \Sigma_{(2\to1)}\phi_{(2)}$$

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

What orthodox theoreticians provide?

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

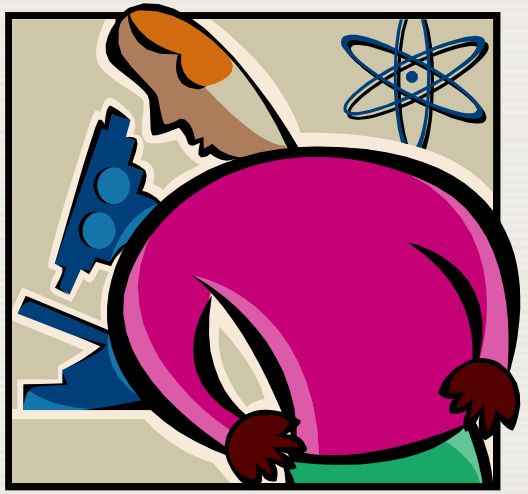


$$\sigma_a(U,J,\pi)=\frac{\pi}{k^2}\frac{(2J+1)}{(2I+1)(2i+1)}\sum_{S=|I-i|}^{I+i}\sum_{l=|J-S|}^{J+S}f(l,\pi)T_l^a(\varepsilon)$$

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 …

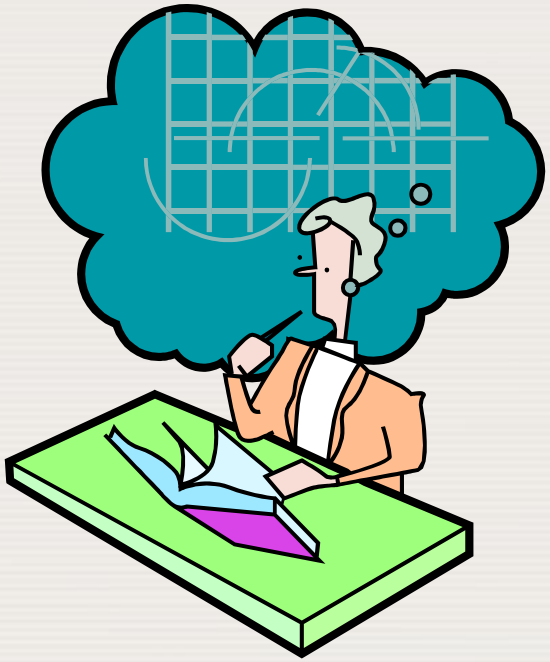
… plot pictures …

Are we there yet?

Nice numbers …

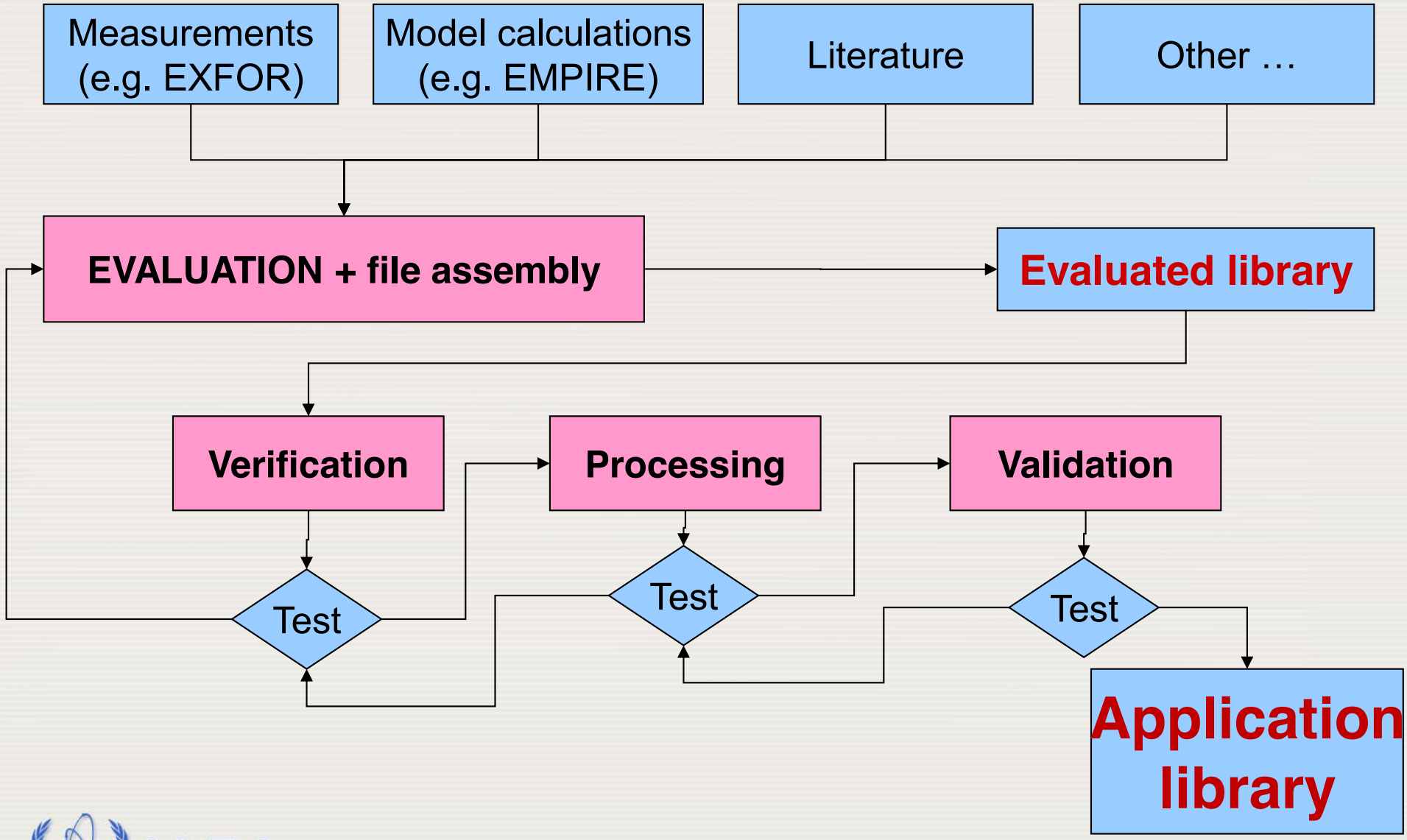
Lots of numbers !

Too many numbers !!!



Besides: which one is right ?

What needs to be done?

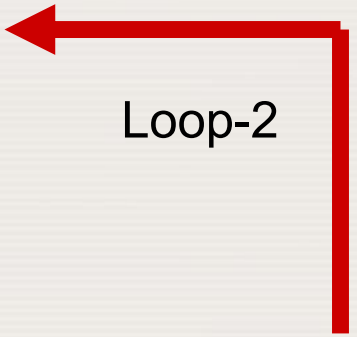


What needs to be done:

- 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

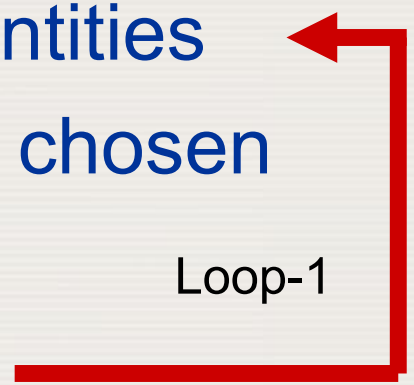
- Evaluation and formatting
- Complete file assembly
- Data file verification
- Processing for applications
- Benchmarking (feedback loop to evaluation)
- Final validation



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



Covariances – fast energy range

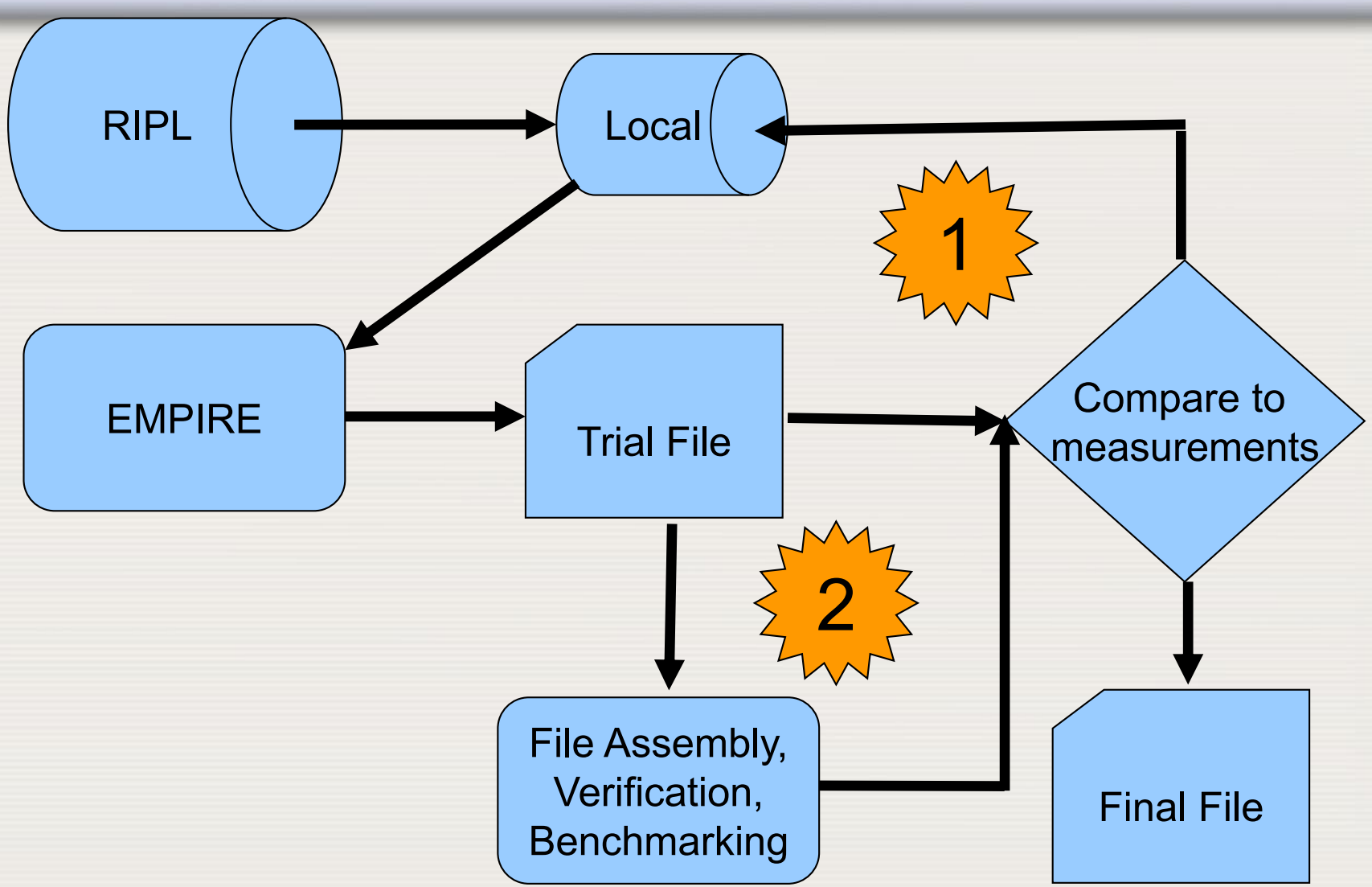
- Prior by random sampling of model parameters within their uncertainties
- Introduce measured data (microscopic cross sections and other quantities) to constrain the uncertainties using Generalised Least-Aquares Method or other (e.g. GANDR)
- Covariances must be consistent with the evaluated cross section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

Evaluated data file assembly

- Data for the resonance and fast range must be assembled consistently (ENDRES)
- Patching into the file covariance data from another evaluation is *dangerous !*


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

Evaluated data storage

- Historical formats
  - (UKNDL, KEDAK, SOKRATOR, ENDL…)
- Current
  - ENDF-6 (adopted worldwide)
- New developments
  - GND (based on XML, being tested)
  - …

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-VI)
- Several releases (updates) may exist (Rel.1)
- Format designation without "/B" and with Arabic numerals for version designation.

ENDF/B-VII Rel.1 – Library from the U.S.A.

ENDF-6 Format (maintained by BNL)

Logical structure of an ENDF file (MF)

1. General information
2. Resonance data
3. Tabulated cross sections
4. Angular distributions (two-body reactions)
5. Outgoing particle emission spectra
6. Coupled angle-energy emission spectra

… Thermal scattering data, photon interactions, etc.

33. Cross section covariance
34. Angular distribution covariances
35. Emission spectra covariances
40. Covariances of partial cross sections (isomer production)

Reaction designation codes (MT)

1. Total
2. Elastic
3. Non-elastic
4. Inelastic
16. Two-neutron emission (n,2n)
17. Three-neutron emission (n,3n)
18. Fission (n,f)

...

51. First discrete inelastic

...

91. Inelastic into continuum
102. Radiative capture (n,g)
103. Proton emission (n,p)

etc

Example 1

```
 MRGMAT files on   Directory of E:\Backup\C\Andrej\data\Tendl-20136000 0  0
 49113.0000 111.934200          2          0          0          14925 1451
 0.0        0.0                 0          0          0          64925 1451
 1.00000000 200000000.          1          0         10       20134925 1451
 300.000000 0.0                 1          0        478        4644925 1451
 49-In-113  NRG       EVAL-NOV13 A.J. Koning and D. Rochman       4925 1451
 TENDL-2013           DIST-      REV1-                           4925 1451
----TENDL-2013        Material 4925         REVISION 1           4925 1451
-----Incident neutron  data                                      4925 1451
------ENDF-6 Format                                             4925 1451
                                                                 4925 1451
TENDL-2013 (TALYS Evaluated Nuclear Data Library)                4925 1451
                                                                 4925 1451
In113 neutron general purpose library                            4925 1451
                                                                 4925 1451
Author: A.J. Koning and D. Rochman, NRG Petten, The Netherlands  4925 1451
                                                                 4925 1451
The TENDL team: A.J. Koning, D. Rochman, S.C van der Marck,      4925 1451
…
…
…
```

Example 2

```
 49113.0000 111.934200          0          0          0          04925 3  1
 0.0        0.0                 0          0          1     1799624925 3  1
     179962           2                                              4925 3  1
 1.00000E-5 614.711740 1.03275E-5 604.894425 1.03345E-5 604.6942524925 3  1
 1.06658E-5 595.234097 1.06801E-5 594.844400 1.10151E-5 585.7283774925 3  1
 1.10373E-5 585.152061 1.13759E-5 576.374715 1.14065E-5 575.6176294925 3  1
 1.17484E-5 567.170724 1.17880E-5 566.237472 1.21332E-5 558.1139384925 3  1
 1.21822E-5 557.013698 1.25306E-5 549.202069 1.25897E-5 547.9376834925 3  1
 1.29410E-5 540.432788 1.30107E-5 539.012251 1.33649E-5 531.8038044925 3  1
 1.34459E-5 530.230656 1.38026E-5 523.312944 1.38956E-5 521.5922964925 3  1
 1.42547E-5 514.957900 1.43603E-5 513.096003 1.47215E-5 506.7366074925 3  1
 1.48406E-5 504.736330 1.52037E-5 498.646838 1.53370E-5 496.5134464925 3  1
 1.57016E-5 490.686565 1.58499E-5 488.425617 1.62159E-5 482.8536594925 3  1
 1.63800E-5 480.469829 1.67470E-5 475.146142 1.69279E-5 472.6424284925 3  1
 1.72955E-5 467.561971 1.74940E-5 464.944607 1.78620E-5 460.0991714925 3  1
 1.80791E-5 457.371541 1.84470E-5 452.755863 1.86838E-5 449.9214714925 3  1
 1.90512E-5 445.530091 1.93087E-5 442.593127 1.96751E-5 438.4200154925 3  1
 1.99545E-5 435.384125 2.03195E-5 431.423746 2.06219E-5 428.2931564925 3  1
 2.09850E-5 424.539486 2.13116E-5 421.318121 2.16723E-5 417.7654484925 3  1
...
```

ENDF-6 Format Features

- Material, data type, reaction – numerical codes MAT, MF, MT (→ dictionary)
- Limited No. of MAT, MF, MT codes
- Fixed format → precision (11 columns)
- Not eye-readable; Manual: "http://www.nndc.bnl.gov/csewg/docs/endf-manual.pdf"

Any new development has to respect the compromise between content and volume…

ENDF-6 Format - Implications

- Computer readability →
  - Processing
- Formal correctness
  - ENDF Checking codes
  - ENDF Pre-Processing codes
- Visualisation
  - On-line and local, e.g. ENDVER package

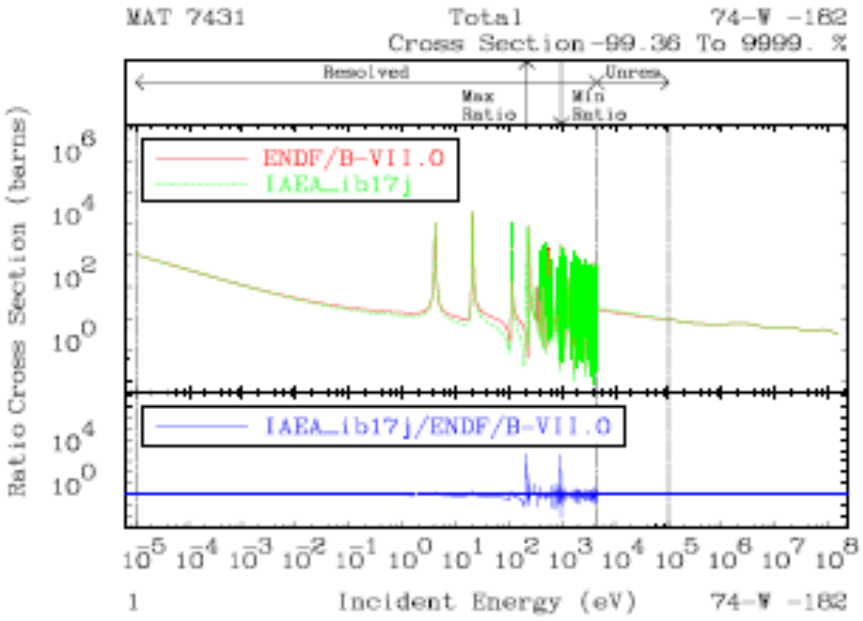
ELEMENTS OF FILE VERIFICATION

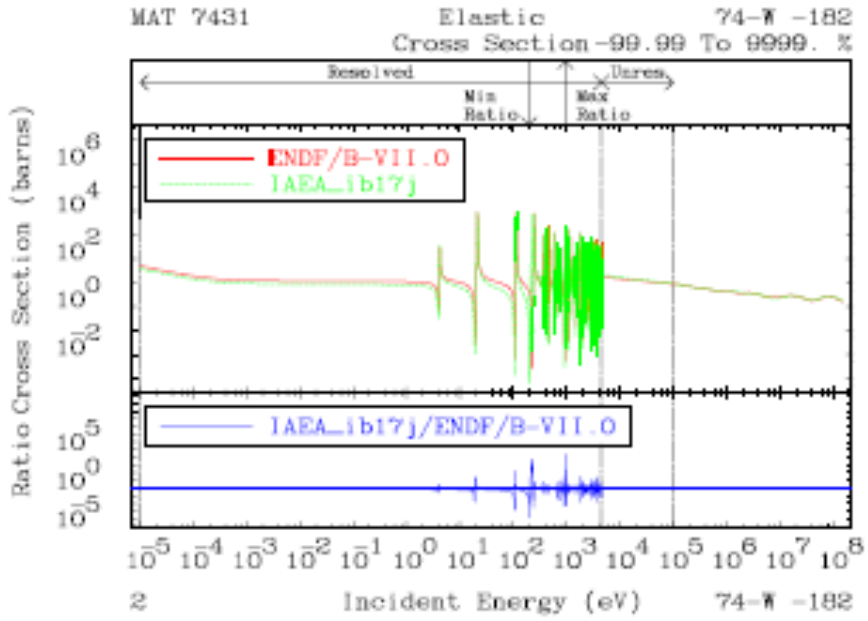
Evaluated file verification

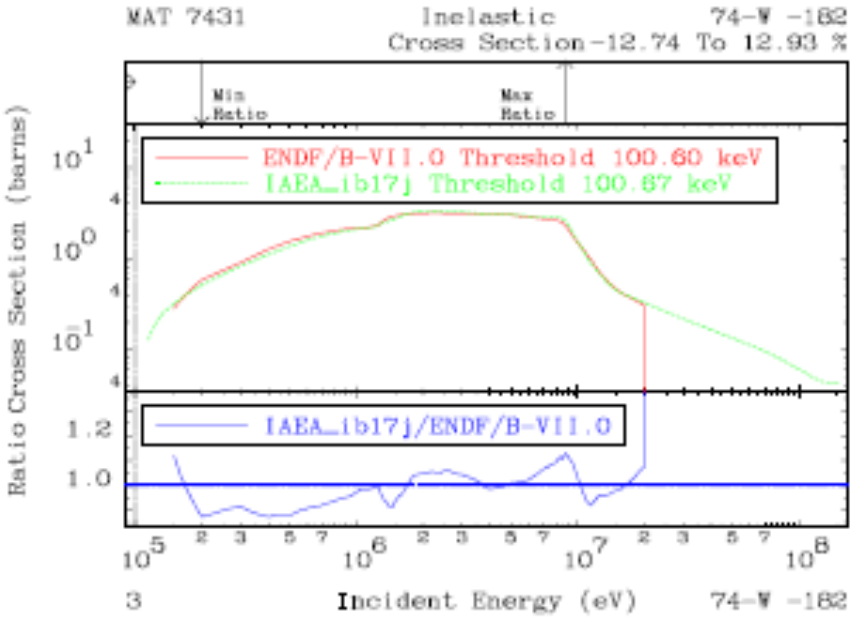
- ENDF Utility codes
  - STANEF: utility to standardise number representation, dictionary, etc.
  - CHECKR: check formal correctness of format
  - FIZCON: check physical consistency of the data
  - PSYCHE: more advanced checking of the file contents

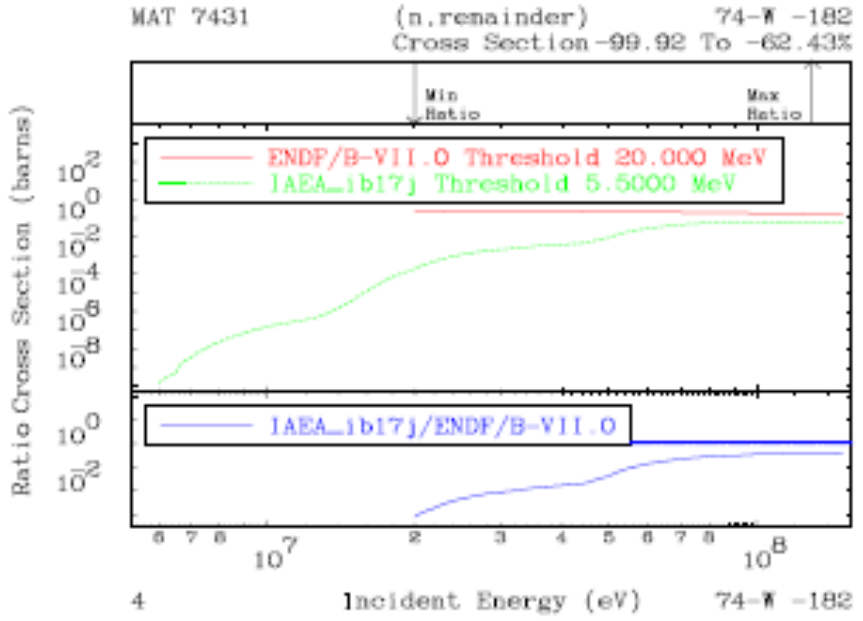
Evaluated file verification (Cont.)

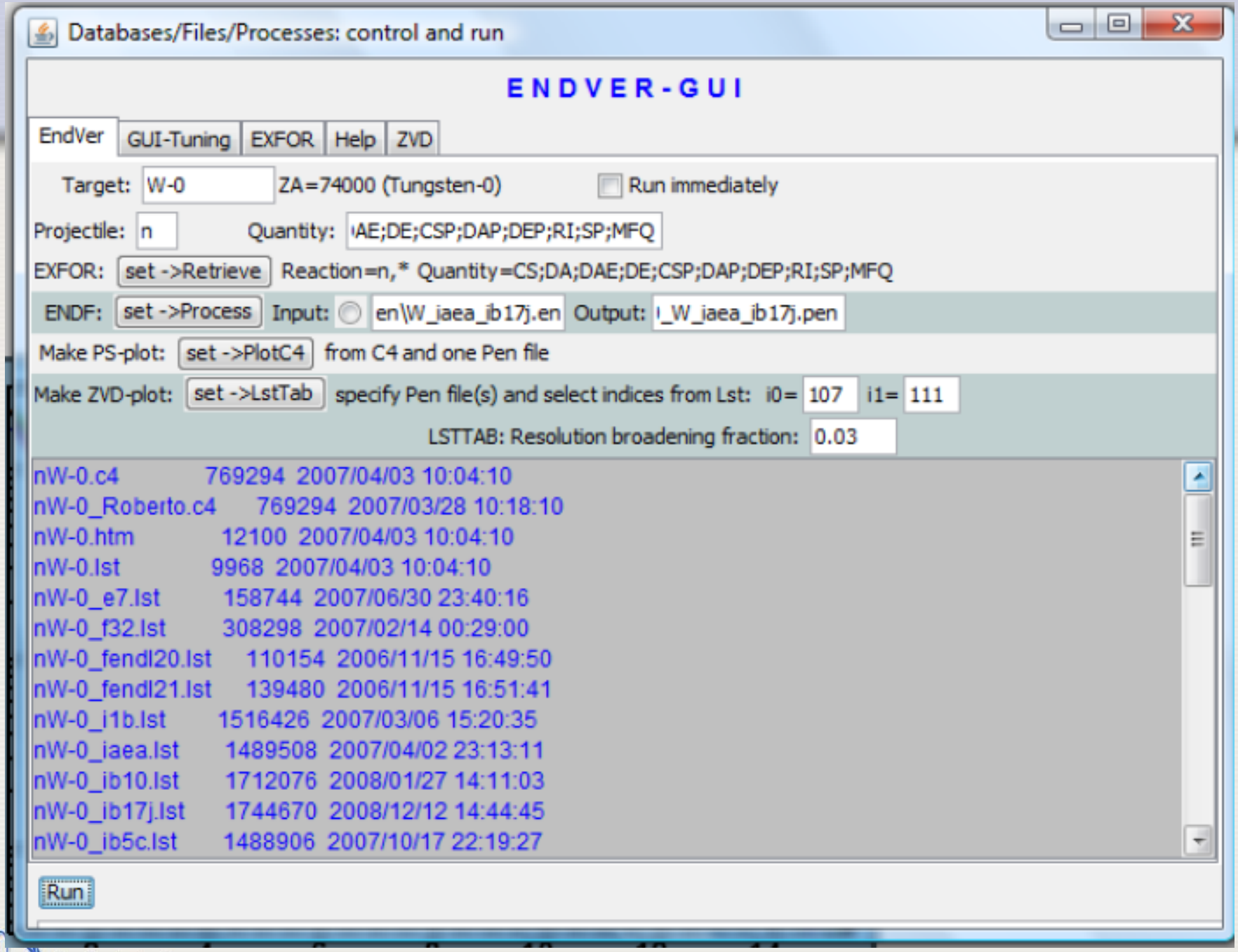
- Pre-Pro ENDF Pre-Processing codes
  - Linearisation, resonance reconstruction, Doppler broadening, etc.
  - First test of data processability.
- ENDVER graphical display package
  - Heavy usage of Pre-Pro and other codes
  - Comparison with experimental data from EXFOR
  - Reconstruction of elemental data from isotopic
  - Reactions defined by summation
  - Differential and double-differential data
- JANIS from the NEA Data Bank …
- On-line data display (IAEA, NEA, NNDC,…)

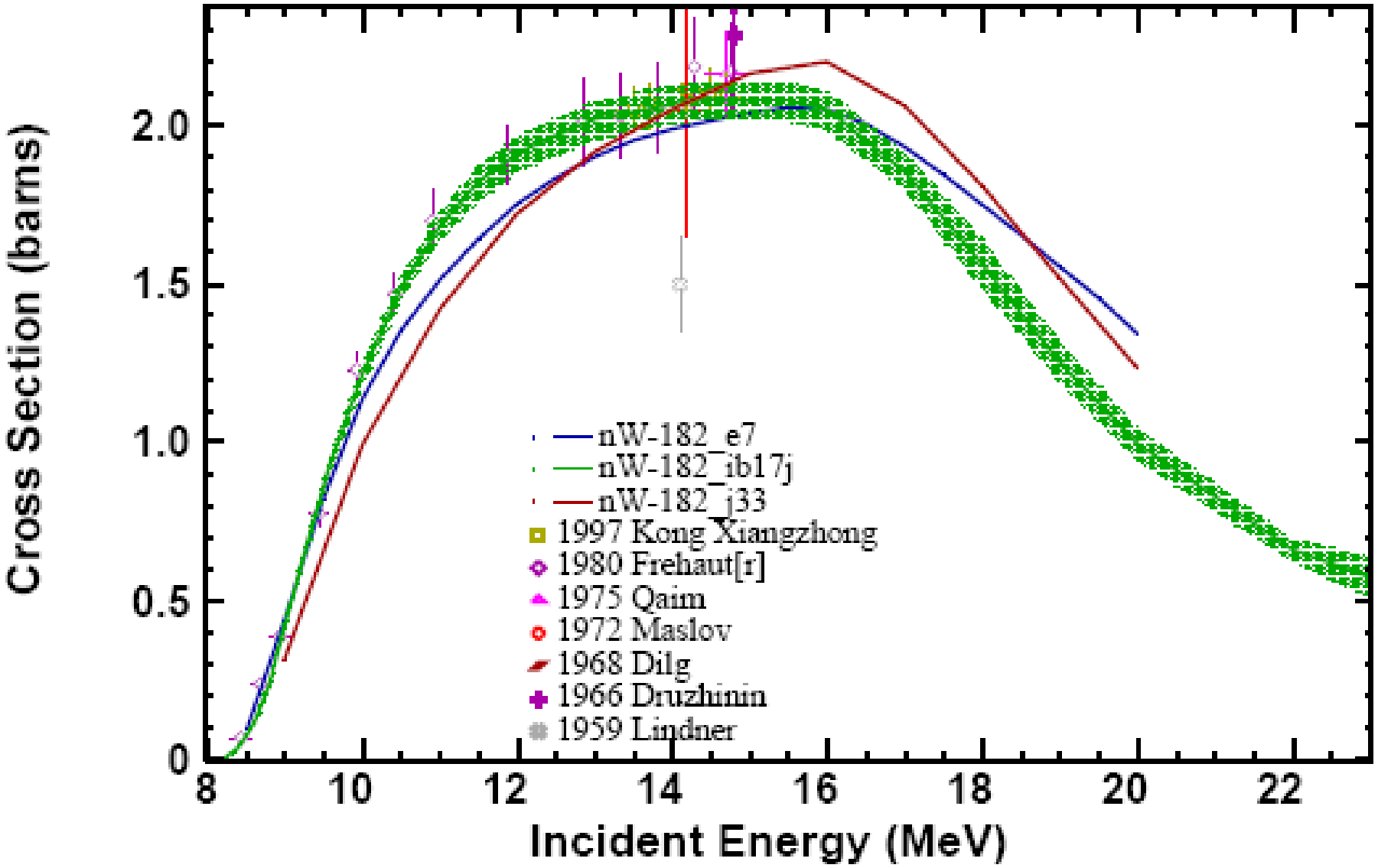

MAT 7431
Total
74-W -182
Cross Section -99.36 To 9999. %
Resolved
Unres
Max Ratio
Min Ratio
ENDF/B-VII.0
IAEA_ib17j
IAEA_ib17j/ENDF/B-VII.0
Ratio Cross Section (barns)
Incident Energy (eV)
1
74-W -182

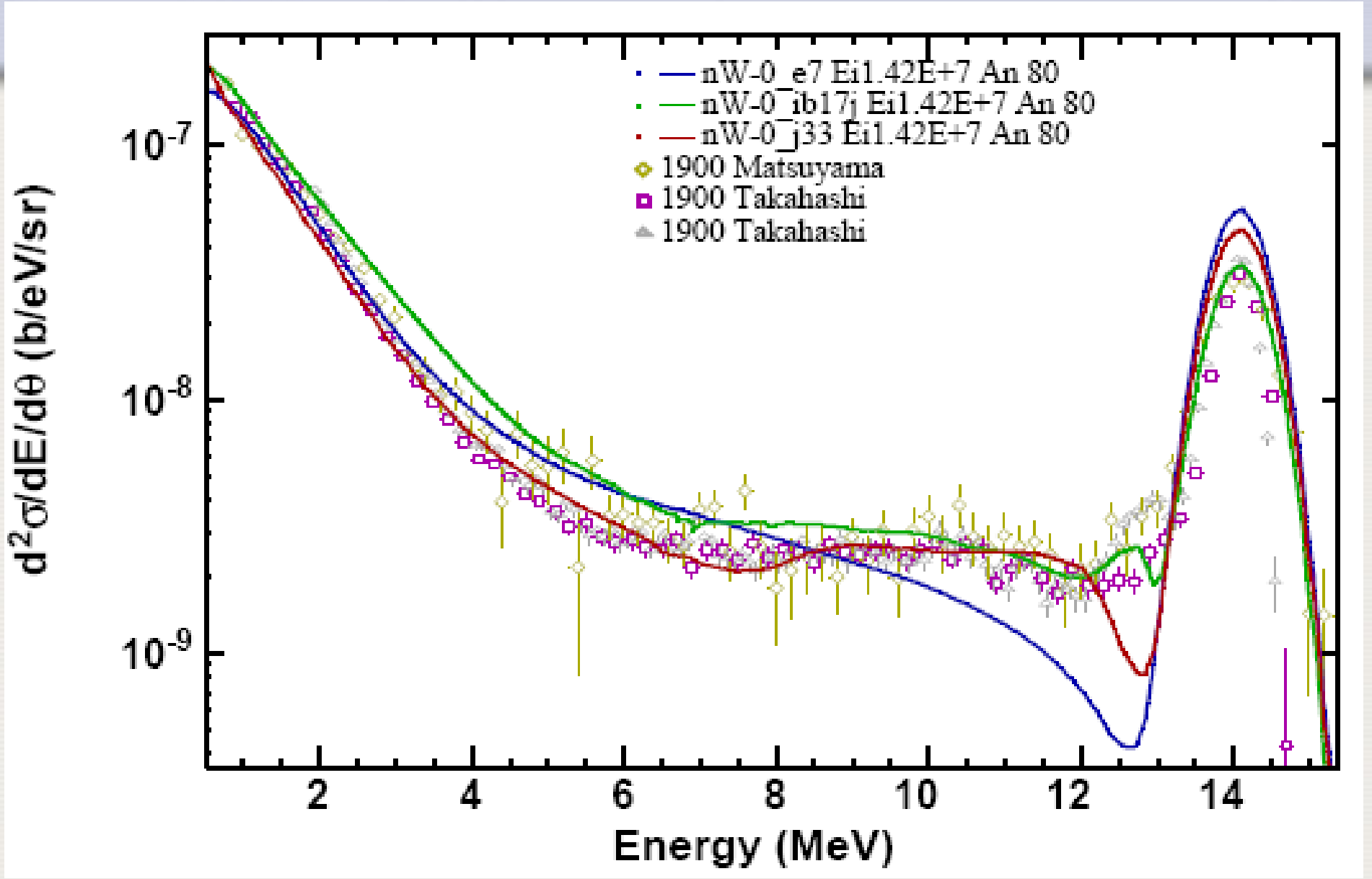

MAT 7431
Elastic
74-W -182
Cross Section -99.99 To 9999. %
Resolved
Unres
Min Ratio
Max Ratio
ENDF/B-VII.0
IAEA_ib17j
IAEA_ib17j/ENDF/B-VII.0
Ratio Cross Section (barns)
Incident Energy (eV)
2
74-W -182


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)
Incident Energy (eV)
3
74-W -182


MAT 7431
(n,renainder)
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)
Incident Energy (eV)
4
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_iaea_ib17j.en
Output: _W_iaea_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_iaea.lst 1489508 2007/04/02 23:13:11
nW-0_ib10.lst 1712076 2008/01/27 14:11:03
nW-0_ib17j.lst 1744670 2008/12/12 14:44:45
nW-0_ib5c.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 for applications

- Monte Carlo transport
  - Mainly re-formatting of cross sections (continuous energy),
  - Self-shielding →probability tables
  - Scattering angular distributions → equi-probable bins
- Deterministic transport
  - Averaging in energy → energy groups (reaction rate conservation)
  - Averaging in space → homogenisation (reaction rate conservation)
- Other
  - Dosimetry (cross sections – pointwise or fine-group)
  - Radioisotope production (pointwise cross sections)
  - Activation (derived composite constants, e.g.: k_0, Q_0)
  - Ion beam analysis (angle-dependent cross sections for incident charged p.)
  - Special applications (fusion, ADS, accelerator shielding – selection of general purpose evaluations, multigroup library in specific format, e.g.: FENDL-3, ADS, WIMS, etc.)

Data Reduction: Group averaging over energy

Reaction Rates

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

Average Cross Sections

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

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

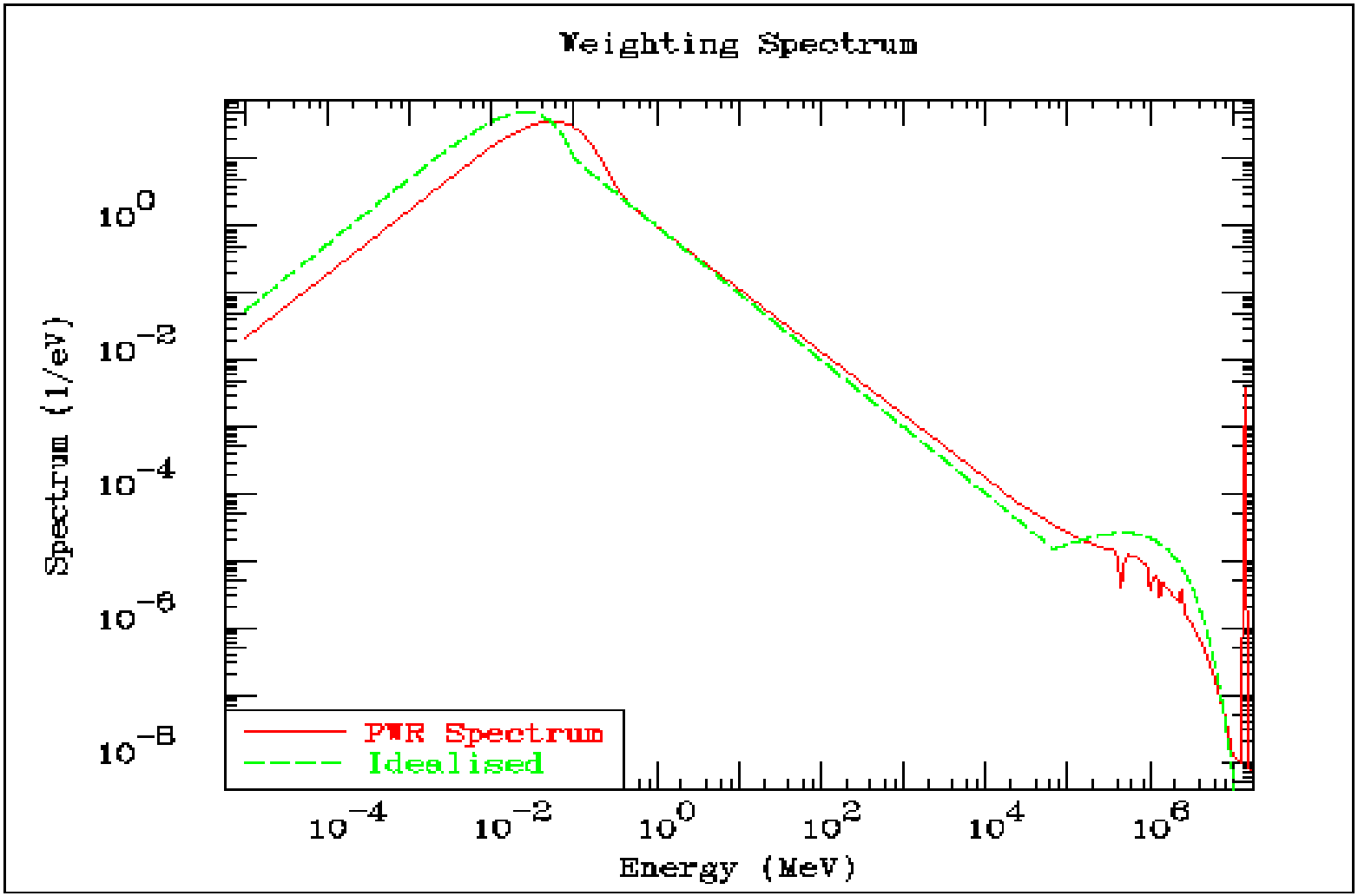
Reaction Rates

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

Average flux and cross sections

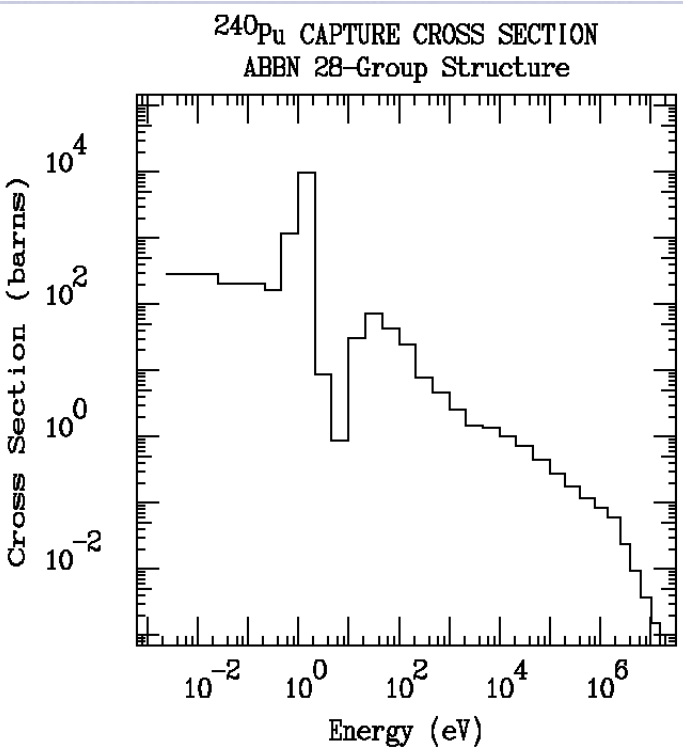
$$\langle \phi_g \rangle = \int_V \phi(\vec{r})dV$$

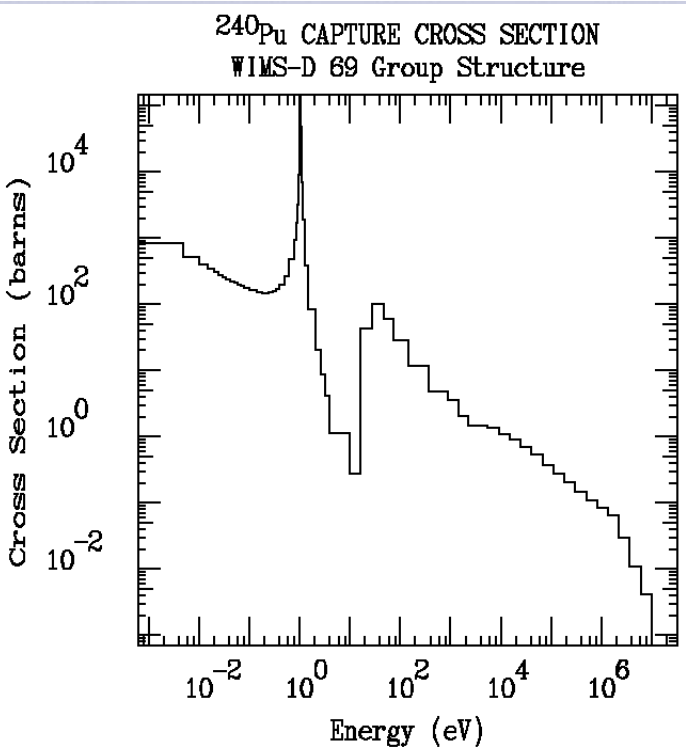
$$\langle \Sigma_g \rangle = \frac{\int_V N\sigma(\vec{r})\phi(\vec{r})dV}{\int_V \phi(\vec{r})dV}$$

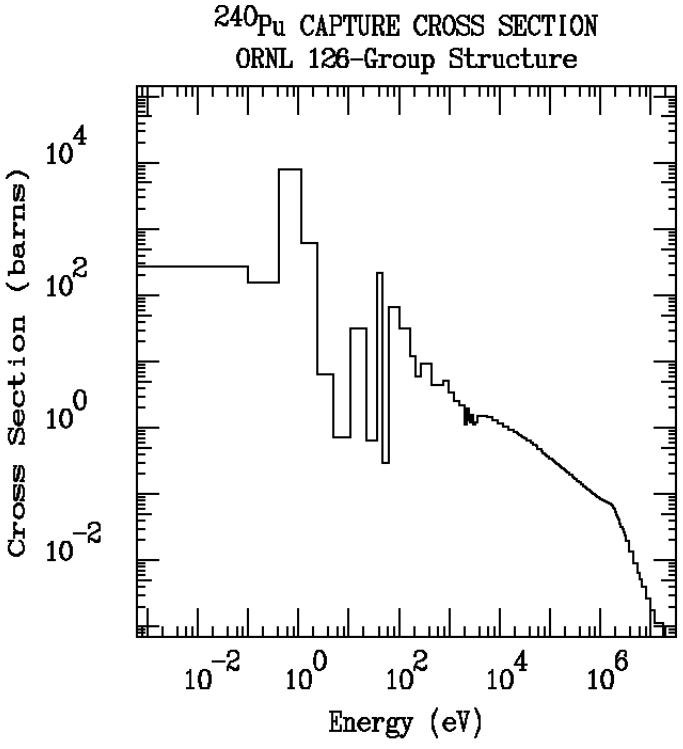

Weighting Spectrum
Spectrum (1/eV)
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
PWR Spectrum
Idealised
10^{-4}
10^{-2}
10^{0}
10^{2}
10^{4}
10^{6}
Energy (MeV)

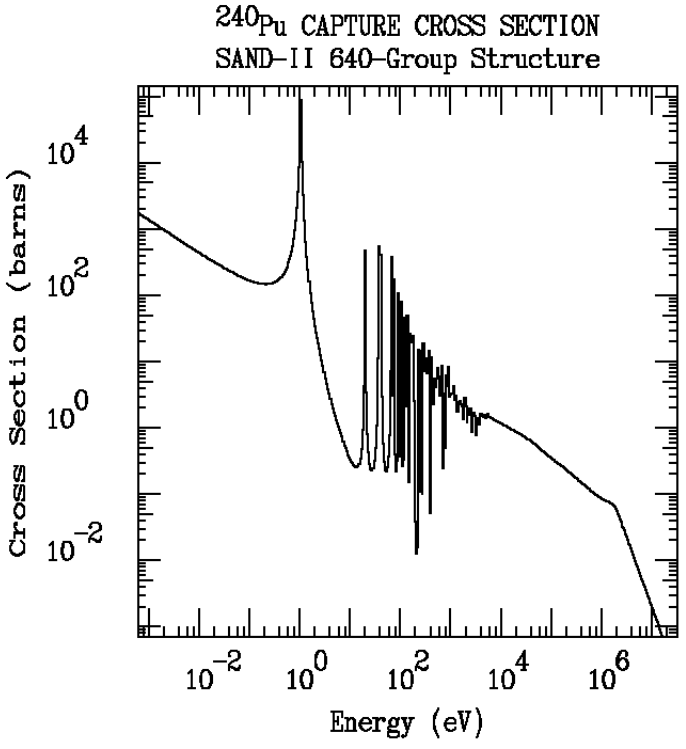
Group averaged data - Definitions

- 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
Cross Section (barns)
Energy (eV)


240Pu CAPTURE CROSS SECTION
WIMS-D 69 Group Structure
Cross Section (barns)
Energy (eV)

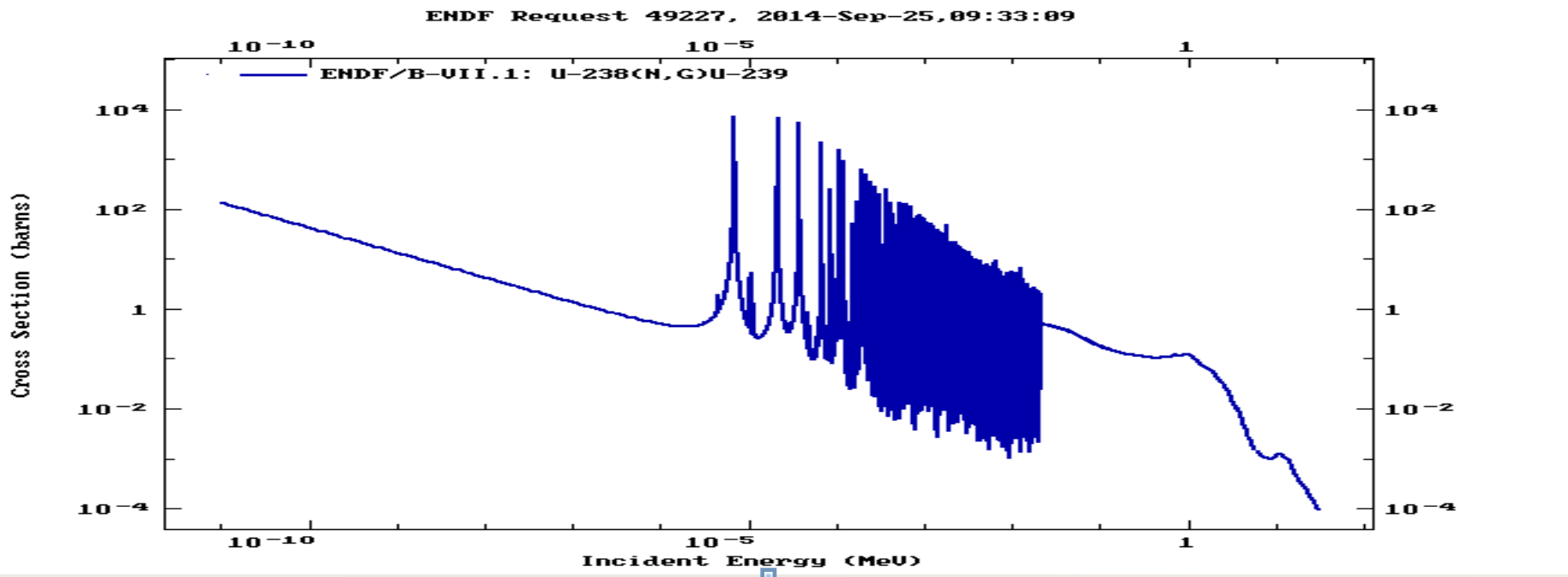

240Pu CAPTURE CROSS SECTION
ORNL 126-Group Structure
Cross Section (barns)
Energy (eV)


240Pu CAPTURE CROSS SECTION
SAND-II 640-Group Structure
Cross Section (barns)
Energy (eV)

Tools - 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 the Los Alamos National Laboratory
- AMPX is a comparable system developed at the Oak Ridge National Laboratory
- Other…

Data reduction – How to ?



How to ?

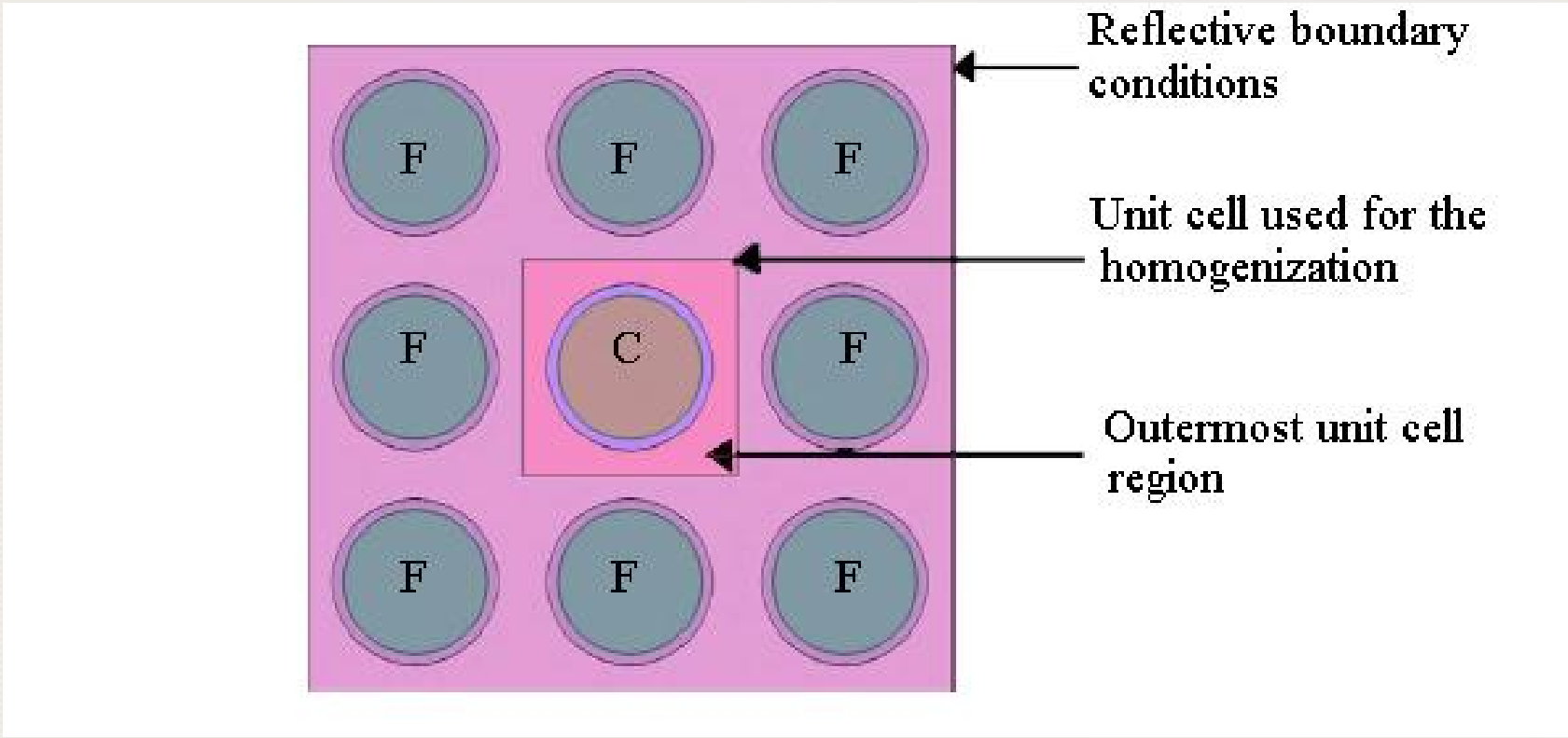
$$-\nabla D_{(1)}\nabla\phi_{(1)} + \Sigma_{a(1)}\phi_{(1)} = \frac{1}{k}\left[\sum_{g}\nu_{(g)}\Sigma_{f(g)}\phi_{(g)}\right] + \Sigma_{(2\to1)}\phi_{(2)}$$

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

Reaction rate conservation

- Averaging equations are exact, but the weighting function is the solution we seek → catch 22
- Proceed in small steps
  1. Fine energy grid (group structure ~26-300 groups), crude geometry (zero-diensional), generic spectrum approximation
  2. Detailed local geometrical model (lattice cell with nearest neighbours), transport solution → homogenised few-group (~4-20 groups) cell cross sections
  3. Coarse mesh geometrical model (fuel assembly with nearest neighbours – one axial slice), transport or diffusion solution → homogenised few-group (~2-4 groups) assembly cross sections
  4. Coarse mesh whole-core model, diffusion solution (thermohydraulic feedbacks, burn-up, reactivity coefficients…)

Lattice cell model



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.)

Benchmark test cases:

- Simple configurations that can be modelled without (significant) simplifications, on which accurate integral measurements were made

Validation:

- Comparison of calculated and measured values

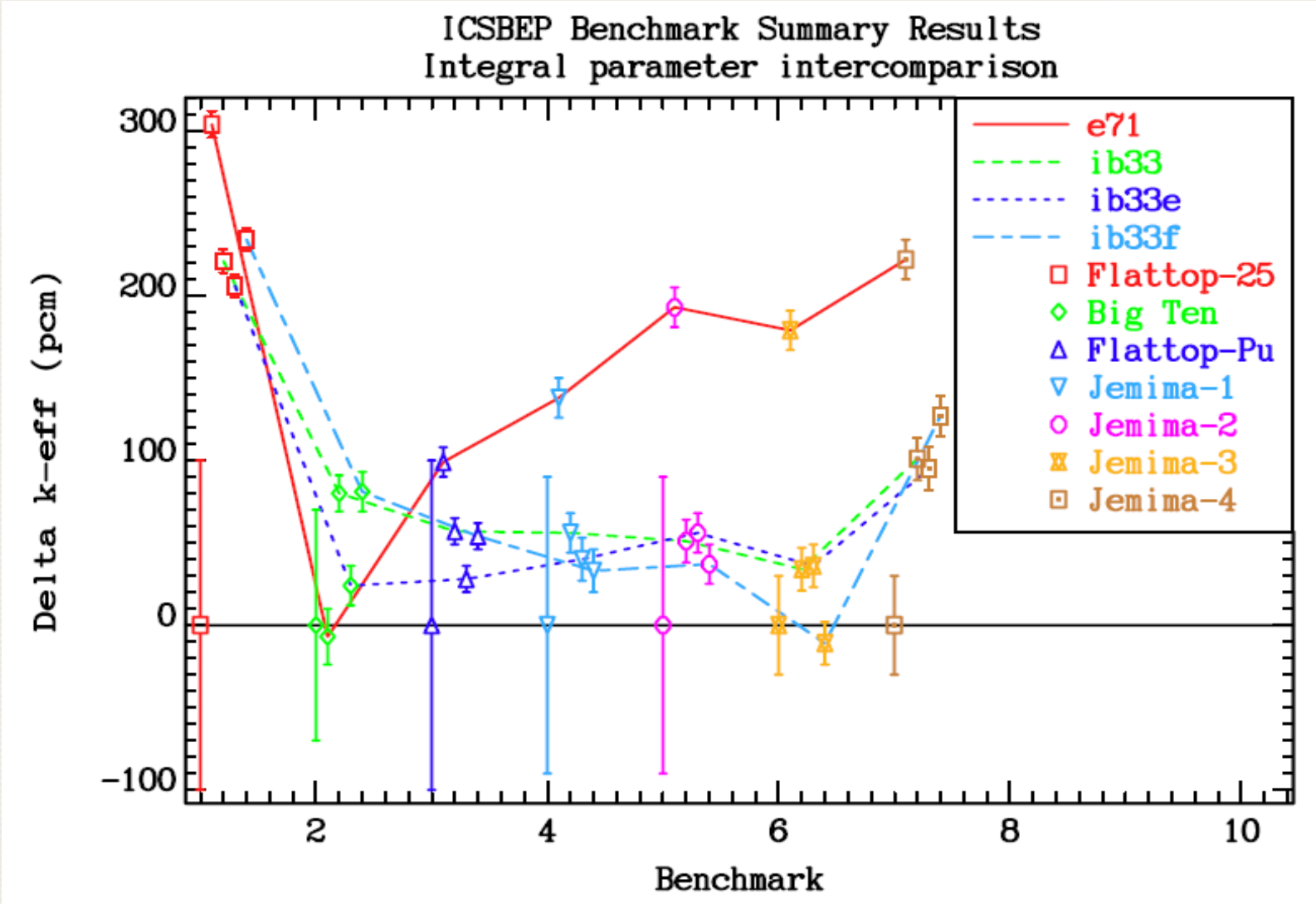
Validity:

- Limited to cases that resemble the benchmark configuration

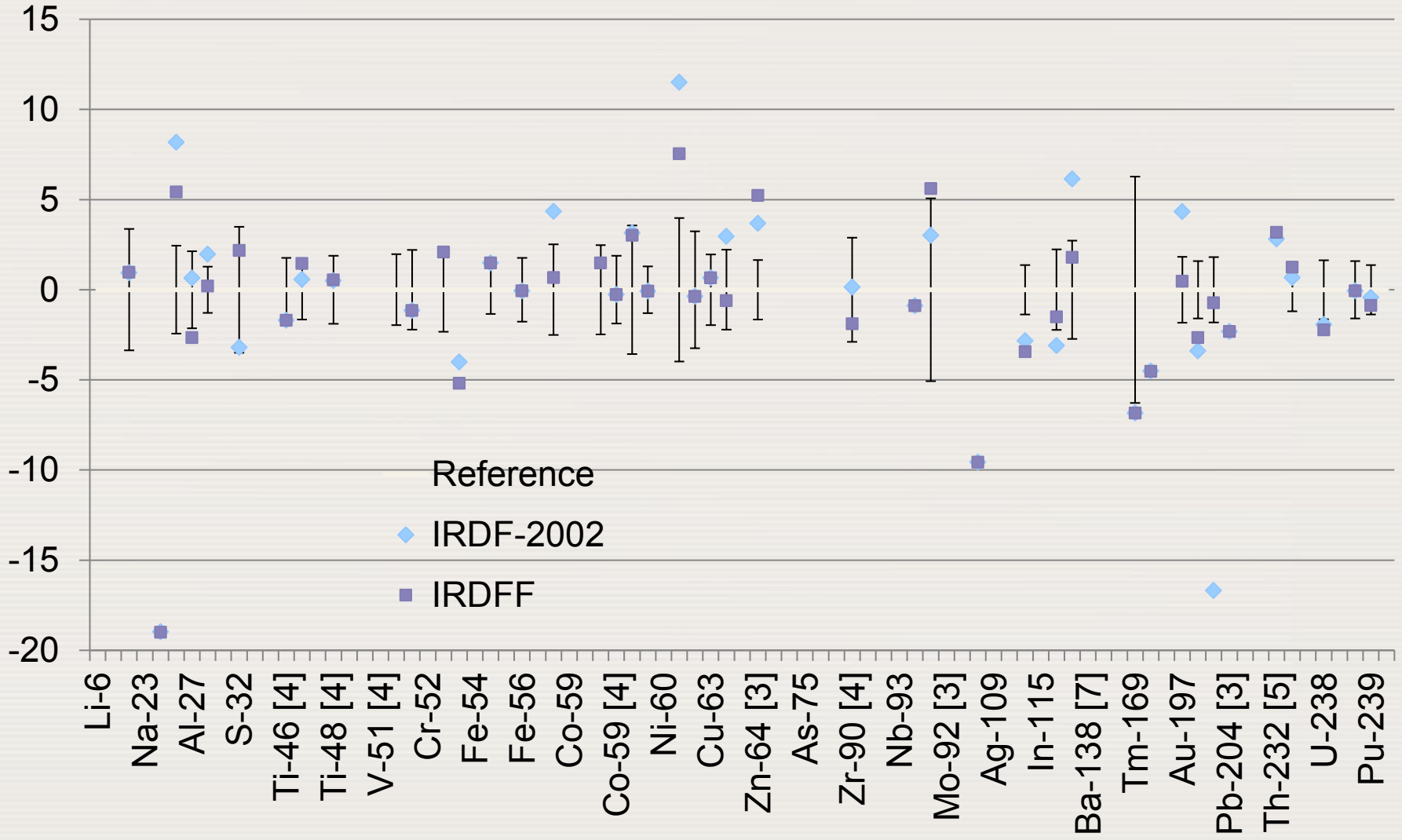
Data validation (Cont.)

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

Example 1


ICSBEP Benchmark Summary Results
Integral parameter intercomparison
Delta k-eff (pcm)
300
200
100
0
-100
2
4
6
8
10
Benchmark
e71
ib33
ib33e
ib33f
Flattop-25
Big Ten
Flattop-Pu
Jemima-1
Jemima-2
Jemima-3
Jemima-4

Example 2: Cf-252 average x.s.



Summary

- Evaluation steps described
- Verification steps defined
- Data reduction (processing) steps described
- Validation:
  - Processing
  - Benchmark calculations
  - (Feedback to evaluation)
  - Validity: cases similar to benchmarks