Simulation codes and data processing tools

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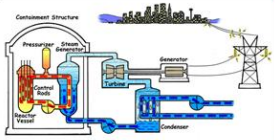
Outline

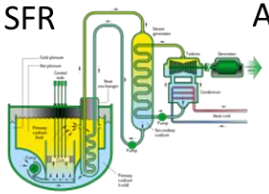
- *Simulation of nuclear applications*
  - *Monte Carlo simulation codes and necessary data*
  - *Deterministic codes and necessary data*
- *Processing of nuclear data: tools and output formats*
- *Basic visualization*
- *Steps in the nuclear data library processing for generations of processed nuclear data libraries: resonances. Doppler broadening, treatment of unresolved resonance region, …*

The importance of Nuclear Data for energy and non-energy applications

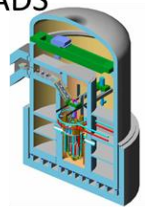
LWR



SFR



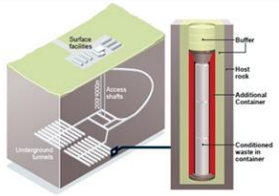
ADS



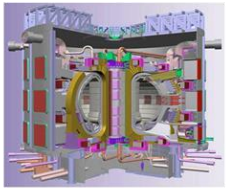
SMRs

Spent Fuel

DGR



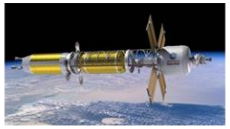
Fusion/ITER



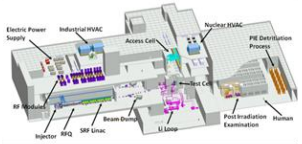
Nuclear Data for Applications (fission and fusion, radiation protection, nuclear medicine, nuclear security, object and materials analysis,…)

and Science (reactions and structure of nuclei, astrophysics, basic physics,…)

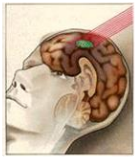
Neutrino's physics



Space technology



IFMIF/DONES



Medical applications

Astrophyscis

Nuclear Data in the modelling

Boltzmann equation: Neutron transport, photon transport, charge particle transport, etc … → criticality, fission power distribution, reactivity coefficients, shielding, spent fuel storage, etc… safety analysis

$$\frac{1}{v}\frac{\partial f}{\partial t}+\mathbf{\Omega}\cdot\nabla f+\Sigma_T f = S+\int dE'd\mathbf{\Omega}'\, f(E',\mathbf{\Omega}')\Sigma_S(E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega})$$

$$S = S_{PF}+S_{dn}+S_{\alpha n}+S_{\text{ext}}$$

$$S_{PF} = \sum_i N_i \int dE'\, f(E')\overline{\nu}_i(E')\sigma_{F,i}(E')f_{P,i}(E',E)$$

$$\Sigma_{S(E\to E',\mathbf{\Omega}\to\mathbf{\Omega}')} = \sum_i N_i \frac{d^2\sigma_{s,i}}{dE'd\Omega'}(E,E',\mathbf{\Omega}\cdot\mathbf{\Omega}')$$

$$\Sigma_T = \sum_i N_i\sigma_{T,i}$$

Doppler ignored

$$\Sigma_T = \Sigma_a+\Sigma_s$$

$$\Sigma_s = \int dE'd\mathbf{\Omega}'\,\Sigma_S(E\to E',\mathbf{\Omega}\to\mathbf{\Omega}')$$

Bateman equation: Inventory evolution, radioactivity, decay heat, dose rates, waste management and environmental impact, etc …

$$\frac{dN_i}{dt} = -\lambda_i N_i - r_i N_i + \sum_{j\neq i}\left\{\lambda_{j\to i}+r_{j\to i}\right\}N_j$$

Modelling for criticality, radiation damage, activation analysis, safegards, reactor emergency core cooling, shielding calculations, radioprotection, ….

Nuclear Data in the modelling

Boltzmann equation: Neutron transport, photon transport, charge particle transport, etc … → criticality, fission power distribution, reactivity coefficients, shielding, spent fuel storage, etc… safety analysis

$$\frac{1}{v}\frac{\partial f}{\partial t}+\mathbf{\Omega}\cdot\nabla f+\Sigma_T f = S+\int dE'd\mathbf{\Omega}'\, f(E',\mathbf{\Omega}')\Sigma_S(E'\to E,\mathbf{\Omega}'\to\mathbf{\Omega})$$

$$S = S_{PF}+S_{dn}+S_{\alpha n}+S_{\text{ext}}$$

$$S_{PF} = \sum_i N_i \int dE'\, f(E')\overline{\nu}_i(E')\sigma_{F,i}(E')f_{P,i}(E',E)$$

$$\Sigma_{S(E\to E',\mathbf{\Omega}\to\mathbf{\Omega}')} = \sum_i N_i \frac{d^2\sigma_{s,i}}{dE'd\mathbf{\Omega}'}(E,E',\mathbf{\Omega}\cdot\mathbf{\Omega}')$$

$$\Sigma_T = \sum_i N_i\sigma_{T,i}$$

Doppler ignored

$$\Sigma_T = \Sigma_a+\Sigma_s$$

$$\Sigma_s = \int dE'd\mathbf{\Omega}'\,\Sigma_S(E\to E',\mathbf{\Omega}\to\mathbf{\Omega}')$$

- Monte Carlo codes: MCNP, SERPENT, OpenMC, MORET, MONK, TRIPOLI, KENO, …
- Deterministic codes: APOLLO, DRAGON, CASMO, NEWT, WIMS10, …

Bateman equation: Inventory evolution, radioactivity, decay heat, dose rates, waste management and environmental impact, etc …

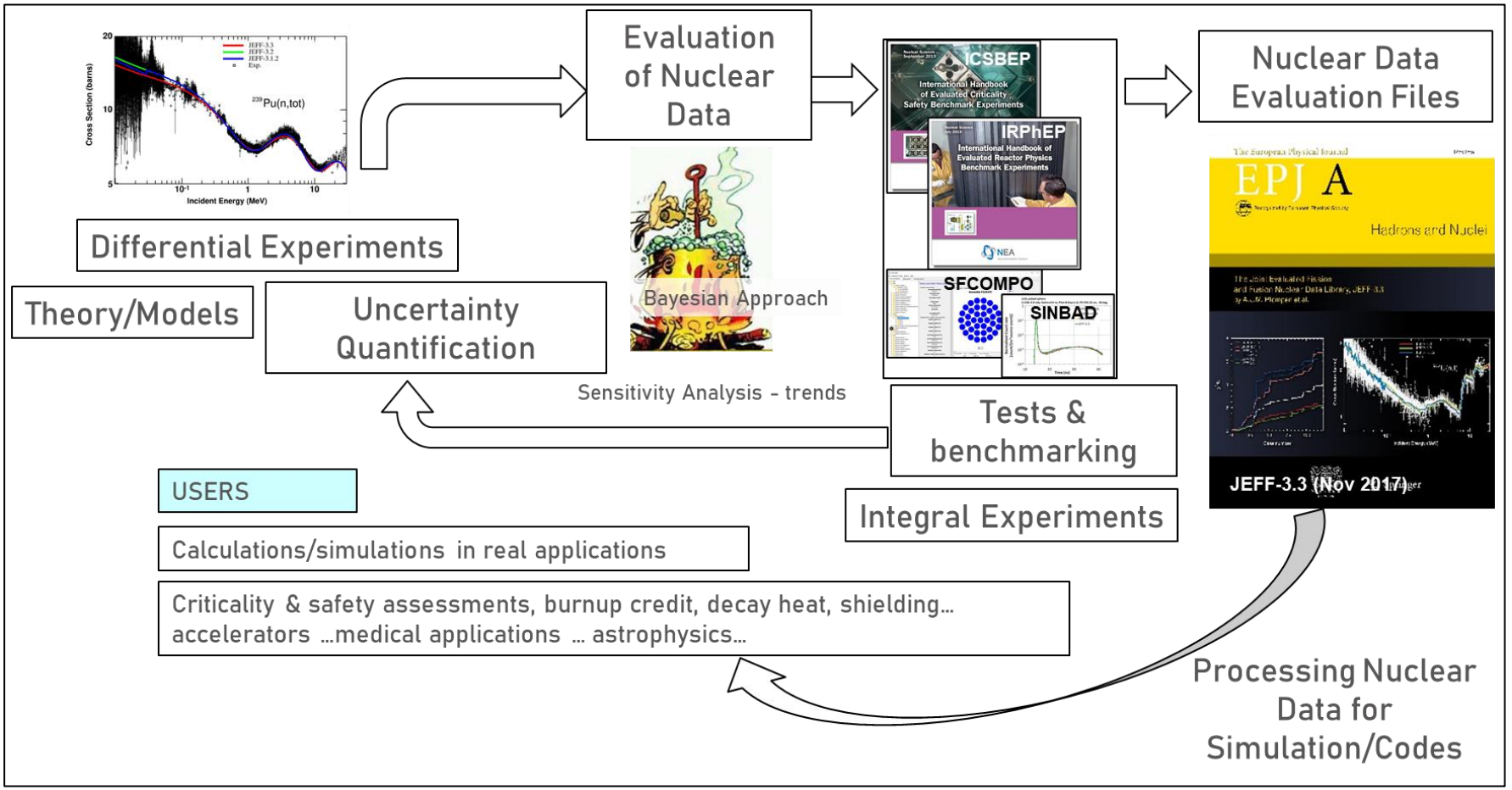
$$\frac{dN_i}{dt} = -\lambda_i N_i - r_i N_i + \sum_{j\neq i}\left\{\lambda_{j\to i}+r_{j\to i}\right\}N_j$$

- Activation codes: FISPACT, ORIGEN, ACAB, DARWIN,…
- Burnup/Depletion codes: EVOLCODE, VESTA, CASMO, SERPENT,…

Modelling for criticality, radiation damage, activation analysis, safegards, reactor emergency core cooling, shielding calculations, radioprotection, ….

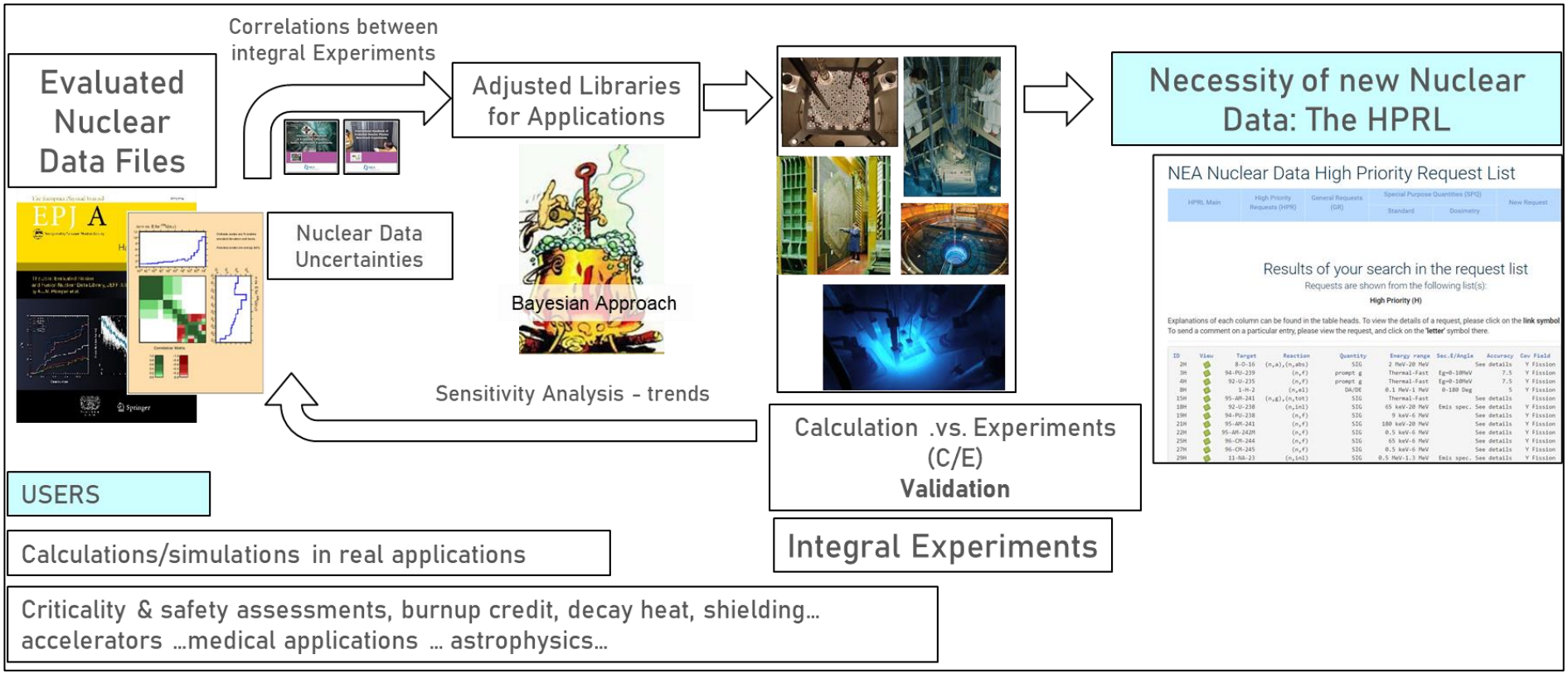
Nuclear Data Cycle

- Nuclear Data are the bridge between the nuclear physics/the differential experiments and the simulations for applications



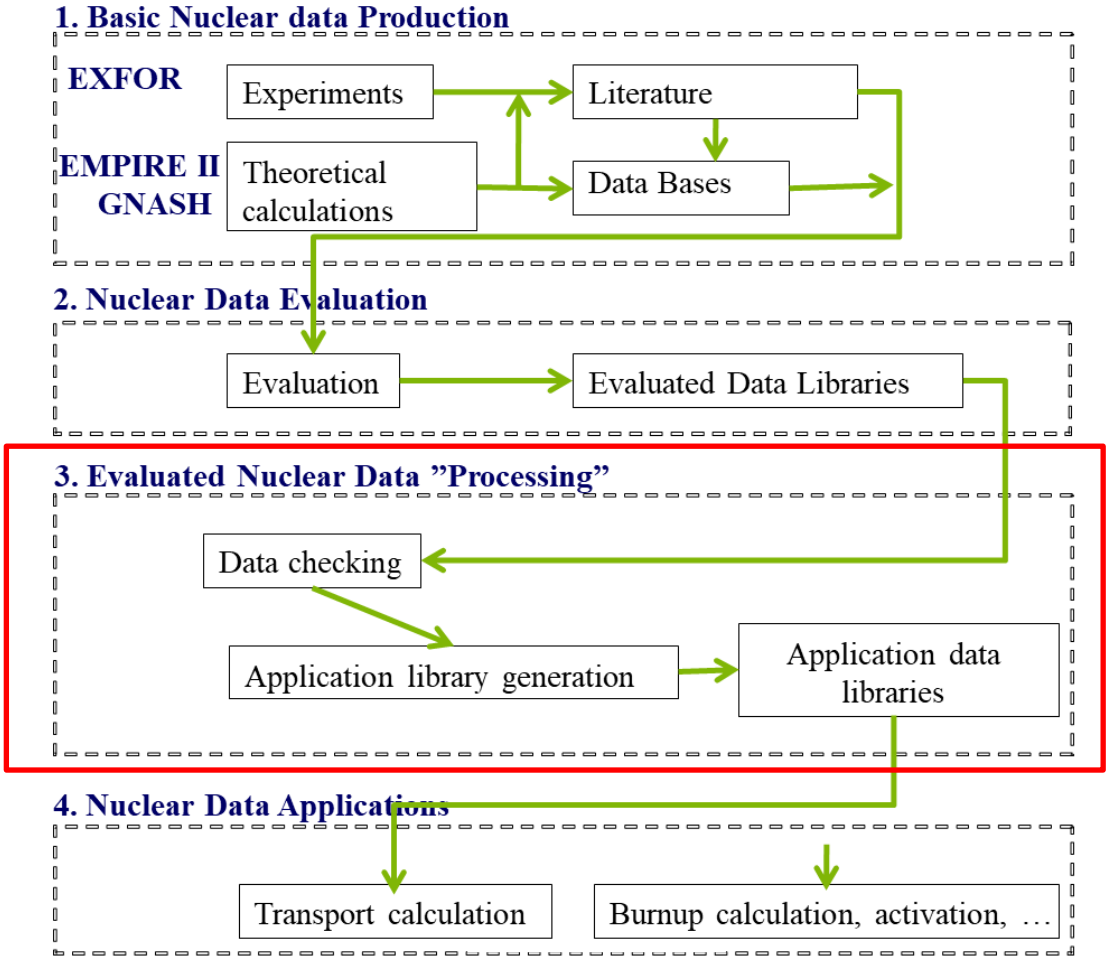
Nuclear Data Cycle

- The End-Users are the bridge between the applications and the necessity of new nuclear data



Nuclear Data Cycle - Pipeline

- Activities associated with Nuclear Data



Processing Codes:
NJOY
CALENDF
PREPRO
AMPX, PUFF
FRENDY, ACEMAKER, …

Ref: A.Trkov. "Status and Perspective of Nuclear Data Production, Evaluation and Validation". Nuclear Engineering and technology, Vol.37 No.1 (2005)

Data checking & verification formats

- ENDF Utility codes for checking data formats and internal consistency developed at NNDC in Brookhaven
  https://www.nndc.bnl.gov/endf/

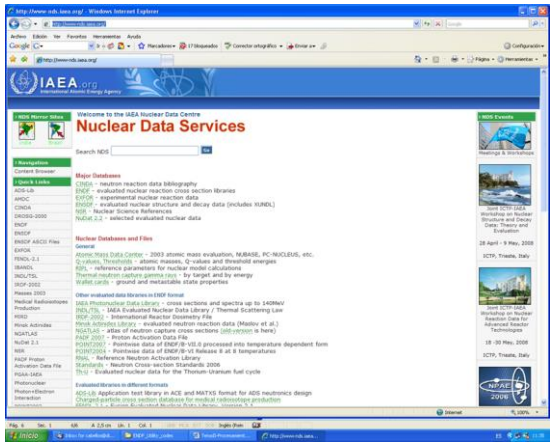
- ENDF Pre-Processing codes of the IAEA: PREPRO2021
  http://www-nds.iaea.org/ndspub/endf/prepro/

- ENDVER package including user-friendly graphics user interface and integrating EXFOR retrieval, ENDF data reconstruction and powerful interactive graphics modules, developed at the IAEANDS
  https://www-nds.iaea.org/public/endf/endver/

- JANIS package + JANIS handbook
  https://www.oecd-nea.org/jcms/pl_39910/janis
  https://www.oecd-nea.org/jcms/pl_44624/janis-books

ENDF Utility Codes

Brief Description	
CHECKR	Format Checking Code
FIZCON	Procedures & Simple Physics Checking Code
PSYCHE	More complicated physics checking code
STANEF	Creates directory, adds tape label & converts numeric fields Converts to binary format
INTER	Calculates selected cross sections and integrals



INTER calculates thermal cross sections, *g-factors*, resonance integrals, fission spectrum averaged cross sections and 14.0 MeV (or other energy) cross sections for major reactions.

g-factor (provides a measure of the deviation from a 1/v shape)
The conventional thermal energy is 0.0253 eV. If the cross section has a 1/*v* shape, its integral weighted against a Maxwellian spectrum for 0.0253 eV is given by

$$I = \int \sigma(E)(E/kT)\exp^{-E/kT} d(E/kT)$$

$$I = \int \sigma(kT)\sqrt{kT/E}\,(E/kT)\exp^{-E/kT} d(E/kT) = \frac{\sqrt{\pi}}{2}\sigma(kT)$$

$$G = \frac{2}{\sqrt{\pi}}\frac{I}{\sigma(kT)}$$

http://www-nds.iaea.org/

http://www-nds.iaea.org/ndspub/endf/utility/index.html

ENDF Pre-Processing codes : PREPRO package

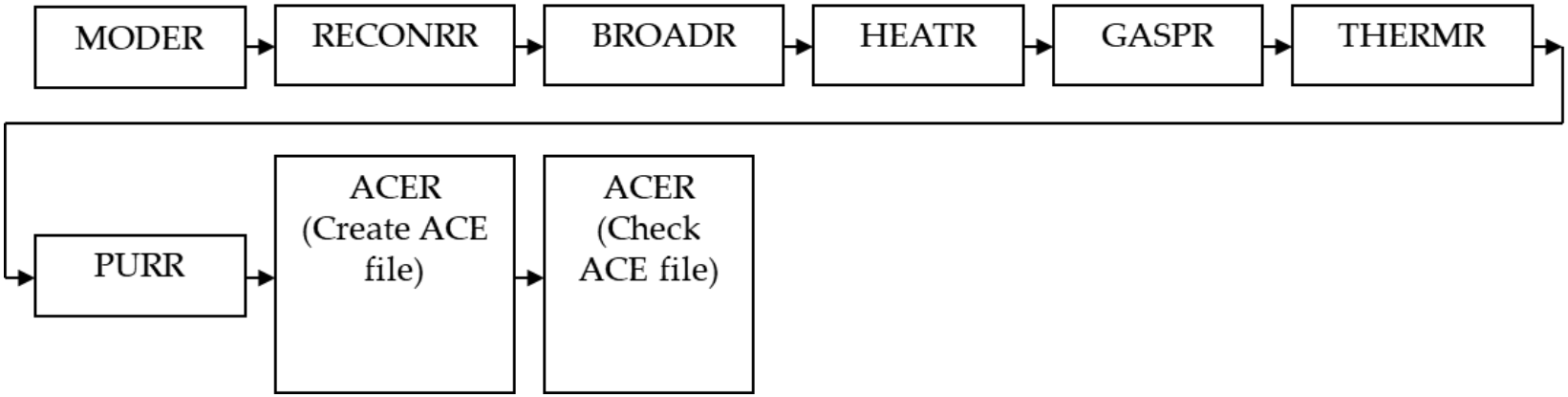
Brief Description	
Linear	Linearize cross sections
Recent	Reconstruct cross sections from resonance parameters
Sigma1	Doppler broaden cross sections
Legend	Calculate/correct angular distributions
Sixpak	Convert double differential data (MF=6) to single differential
Fixup	Correct format and cross sections, define cross sections by summation
Dictin	Create reaction dictionary (MF=1, MT=451)
Merger	Retrieve and/or Merge evaluated data
Groupie	Calculate group averages and multi-band parameters
Complot	Plot comparisons of cross sections (MF=3, 23); Comhard for hardcopy
Evalplot	Plot evaluated data (MF=3, 4, 5, 23, 27); Evalhard for hardcopy
Mixer	Calculate mixtures of cross sections
Convert	Convert codes for computer/precision/compiler
Relabel	Relabel and sequence programs
…	…

http://www-nds.iaea.org/ndspub/endf/prepro

NJOY Processing System

- NJOY is a comprehensive system for generating application libraries, developed at Los Alamos National Laboratory.

Figure: Example of sequential NJOY modules to process ACE (MCNP) files



https://github.com/njoy/NJOY2016

https://github.com/njoy/NJOY21

NJOY modules

Brief Description		
MODER	Converts ENDF "tapes" back and forth between ASCII format and the special NJOY blocked-binary format	← Input ENDF tape
RECONR	Reconstruct pointwise cross sections from endf/b resonance parameters and interpolation schemes	→ Output PENDF
BROADR	Doppler broaden and thin pointwise cross sections	→ Output PENDF
GROUPR	Generate self-shielded multigroup cross sections and group-to-group scattering and photon production matrices	→ Output GENDF
ERRORR	Construct multigroup covariance matrices	
COVR	Process covariance data from error	
ACER	Prepare library for the Los Alamos continuous energy monte-carlo code MCNP	→ Output ACE/xdir
WIMSR	Convert multigroup data into libraries for the reactor assembly codes wims-d or wims-e	→ Output WIMSD
PLOTR	Plot endf, pendf, gendf, or exp. cross sections, distributions, or matrices	
VIEWR	View plots from plotr, dtfr, covr, etc. in postscript	
PURR	Generate unresolved-resonance probability tables for the MCNP code	
…	…	

NJOY modules

❑ MODER

- Copy a tape from ascii/binary format to binary/ascii
- Extract an individual material from a multi-material tape and copy (including ascii/binary or binary/ascii conversion) to a new tape
- Create a custom multi-material tape (including ascii/binary or binary/ascii conversion)
- Strongly recommend that MODER be the first module executed by the User, to create a binary tape

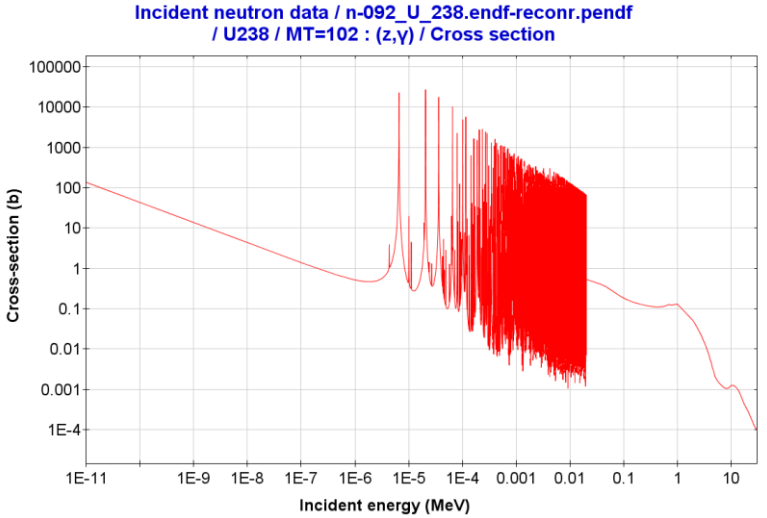
```
moder / Extract/convert neutron evaluated data
1 -21
'92-U-235 from JEFF3.1'/
20 9228
0/
```

NJOY modules

❑ RECONR

- Resonance reconstruction, linearization, grid unionization, derived cross sections …
- Resonance reconstruction …
  - ENDF formats allow the evaluator to define a variety of RR formats (LRF #).
    - SLBW (1), MLBW (2), Reich-Moore (3), Adler-Adler(4), General R-Matrix (5), Hybrid R-Function (6), Limited Reich-Moore (7).
    - SLBW only appears in old evaluations, MLBW used for many non-actinides, R-M in modern actinide evaluations, LRF=7 is relatively new (ENDF/B-VII.1 35Cl; CIELO 56Fe, maybe 16O).
- **Linearization:** Add energy points so that linear-linear interpolation reproduces the original interpolation to within a User specified tolerance (typically 0.1%)

```
reconr
 -21 -22/                    card 1
 'tape id after reconr'/     card 2
 9237/                       card 3
 0.01/                       card 4
 0/
```

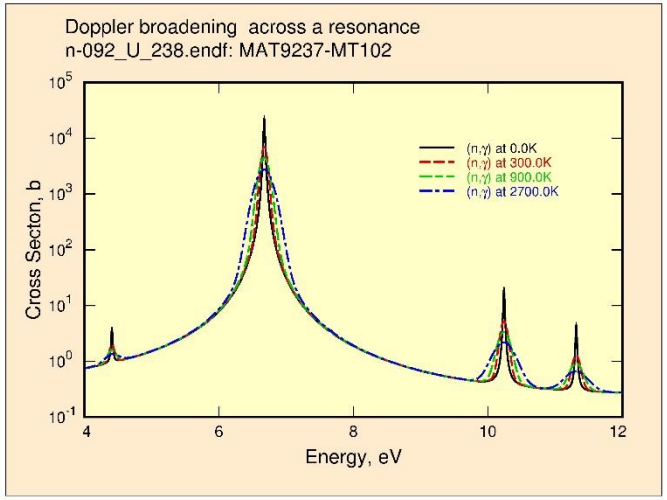


NJOY modules

❑ BROADR

- Doppler broadening
  - User specifies the initial temperature and final temperature
  - Energy mesh reconstruction tolerances can differ from those used by RECONR
  - Some characteristics of Doppler broadened cross sections …
    - 1/v cross sections are invariant;
    - constant cross sections develop a 1/v tail;
    - resonance peaks decrease and broaden.
    - usually have fewer energy mesh points after Doppler broadening

```
broadr
 -21 -22 -23/                  card 1
 9237 3/                       card 2
 0.01/                         card 3
 300.0 900.0 2700.0            card 4
 0/                            card 5
```

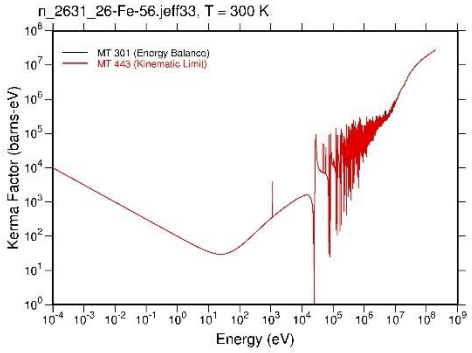


NJOY modules

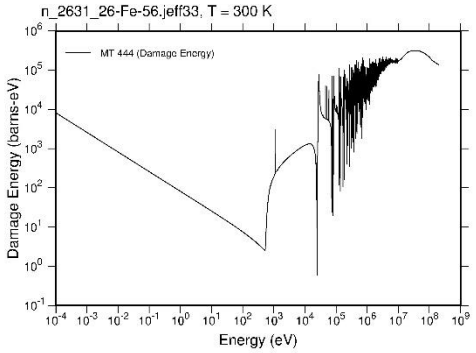
❑ HEATR: Total Heating, Heating by Reaction, Radiation Damage

- Heating is described using “KERMA” (Kinetic Energy Release in Materials),
- Radiation Damage has many sources … direct heating, gas production, lattice defect production. Atomic displacement depends upon total available energy and the energy required to displace an atom …

```
heatr    /
 -21 -25 -26 45   /
  2631 7 0 0 0 1    /
 303 304 318 443 444 445 447 /
```




```
MT=302:   Elastic
MT=303:   Non-elastic
MT=304:   Inelastic
MT=318:   Fission
MT=402:   Capture
MT=443:   Total kinematic kerma
MT=444:   Total damage energy production
```



NJOY modules

❑ UNRESR

- To produce effective self-shielded cross sections in URR for deterministic transport codes
- ENDF-6 files provide average values for resonance widths and spacings together with distribution functions for the widths and spacings
- UNRESR converts this representation into effective cross sections (total, capture, fission or elastic) suitable for codes that use the background cross section method(the Bondarenko method)

$$\bar{\sigma}_{0x}(E^*) = \frac{\int_{E_1}^{E_2} \sigma_x(E)\varphi_0(E)dE}{\int_{E_1}^{E_2} \varphi_0(E)dE}$$

φ_0 is scalar flux, E* is the effective energy in $[E_1,E_2]$ where cross sections are slowly varying with E

$$\bar{\sigma}_{1t}(E^*) = \frac{\int_{E_1}^{E_2} \sigma_t(E)\varphi_1(E)dE}{\int_{E_1}^{E_2} \varphi_1(E)dE}$$

φ_1 is P_1 component of neutron flux proportional to neutron current

Shape of flux:

$$\varphi_l(E) = \frac{C(E)}{[\Sigma_t(E)]^l} = \frac{C(E)}{[\sigma_0 + \sigma_t(E)]^l}$$

- σ_0 is the parameter that controls the depth of the resonance dips in the flux.
- Infinite dilution: $\sigma_0 = 10^{10}$ b

NJOY modules

GROUPR

- Computes multigroup cross sections, group-to-group scattering matrices, and anisotropic photon production matrices for neutrons
- Bondarenko narrow-resonance weighting scheme

$$\langle \Sigma_X \rangle_g = \frac{\int_{Eg}^{Eg+1} \Sigma_X(E)\omega(E)dE}{\int_{Eg}^{Eg+1} \omega(E)dE}$$

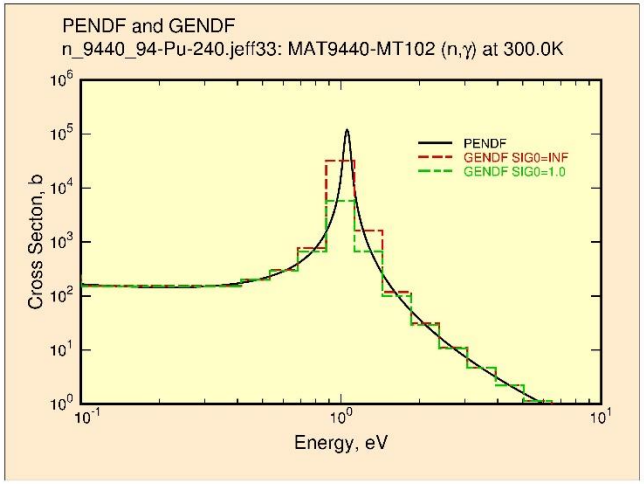
```
groupr
-21 -24 0 35 /
9440 17 0 2 1 1 2 1 /
'Pu240 IGN=17 T=300.0K Sig0s'/
300.0
1.e10 1.e+0
3 /
0/
0/
```

Table: Standard neutron group structures

ign	meaning
1	arbitrary structure (read in)
2	csewg 239-group structure
3	lanl 30-group structure
4	anl 27-group structure
5	rrd 50-group structure
6	gam-i 68-group structure
7	gam-ii 100-group structure
8	laser-thermos 35-group structure
9	epri-cpm 69-group structure
10	lanl 187-group structure
11	lanl 70-group structure
12	sand-ii 620-group structure
13	lanl 80-group structure
14	eurlib 100-group structure
15	sand-iia 640-group structure
16	vitamin-e 174-group structure
17	vitamin-j 175-group structure
18	xmas nea-lanl
19	ecco 33-group structure
20	ecco 1968-group structure
21	tripoli 315-group structure
22	xmas lwpc 172-group structure
23	vit-j lwpc 175-group structure

Table: Standard weight function options

iwt	meaning
1	read in smooth weight function
2	constant
3	1/e
4	1/e + fission spectrum + thermal maxwellian
5	epri-cell lwr
6	(thermal) – (1/e) – (fission + fusion)
7	same with t-dep thermal part
8	thermal–1/e–fast reactor–fission + fusion
9	claw weight function
10	claw with t-dependent thermal part
11	vitamin-e weight function (ornl-5505)
12	vit-e with t-dep thermal part
-n	compute flux with weight n
0	read in resonance flux from ninwt



NJOY modules

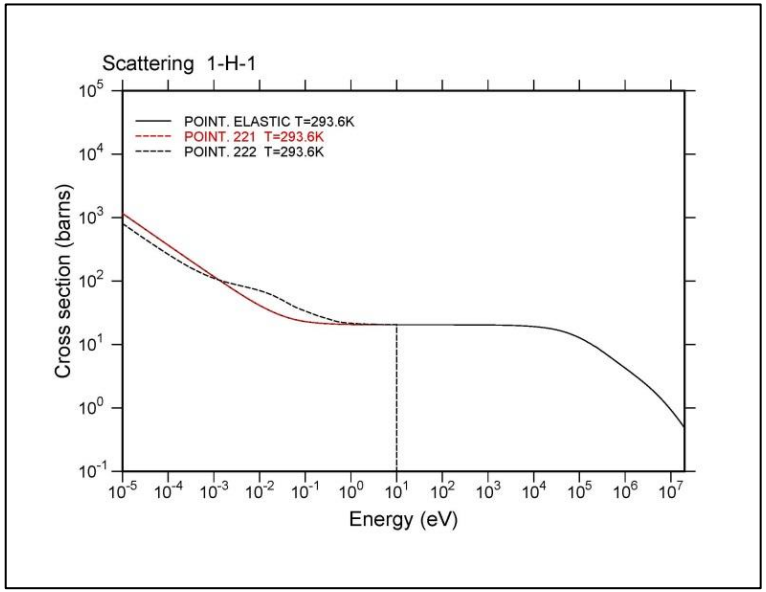
❑ THERMR

- Produce cross sections and energy matrices for free or bound scatters at thermal energies

```
thermr / Add thermal scattering data (free gas)
0 -24 -62
0  125  20 1 1 0 0 2 221 1 / free-gas model(mt=221)
293.6 /
0.001 10.0 / tolerance emax)
thermr / Add thermal scattering data (bound)
 -61 -62 -27
1 125 20 1 2  0 0 2 222 1/
293.6 / Temp. in K
0.001 10.0 /
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .32/ LOPT=2, ".32"=suffix
'H-H2O   293.6 K from NEA_OCT2016'/
125 293.6 'lw00  ' /
 1001    0    0 /
 222 64   0  0  1 10.0 0/
acer / Check ACE files
0 28 0 71 81
7 1 1 -1/
/
stop
```

Table. Moderator materials available for ENDF/B-VII thermal data files showing their MAT numbers and the special MT numbers used by NJOY.

Material	MAT	MTs	elastic	secondary
Al	45	243,244	coh	
Be	26	231,232	coh	
Be(BeO)	27	233,234	coh	
O(BeO)	28	237,238	coh	
C(graphite)	31	229,230	coh	
Fe	56	245,246	coh	
H(CH_2)	37	223	iel	free C
H(liquidCH_4)	33			
H(solidCH_4)	34			
C_6H_6	40	227		none
D(D_2O)	11	228		free O
D(paraD_2)	12			
D(orthoD_2)	13			
H(H_2O)	1	222		free O
H(paraH_2)	2			
H(orthoH_2)	3			
Zr(ZrH_n)	58	235,236	iel	
H(ZrH_n)	7	225,226	iel	
U(UO2)	76	241,242	coh	
O(UO2)	75	239,240	coh	

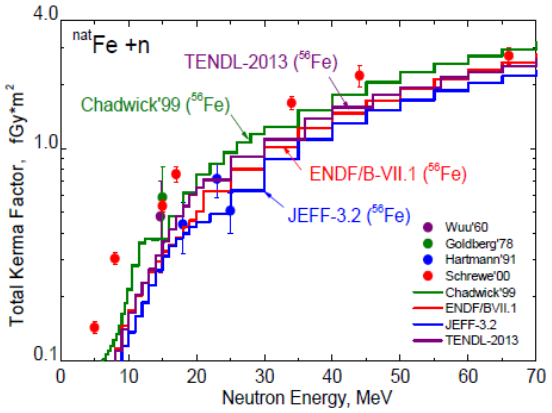


NJOY modules

```
c     *  mixr                                                      *   mixr.
c     *                                                            *   mixr.
c     *  construct a new pendf tape with a specified set of        *   mixr.
c     *  reactions that are specified linear combinations of the   *   mixr.
c     *  cross sections from the input tapes.  mixr can also be    *   mixr.
c     *  used for endf tapes, but the input interpolation laws     *   mixr.
c     *  are ignored.  this module can be used to construct mixed  *   mixr.
c     *  reactions for plotting (for example, elemental cross      *   mixr.
c     *  sections).  the output file contains files 1 and 3 only.  *   mixr.
c     *  linear-linear interpolation is assumed.                   *   mixr.
c     *                                                            *   mixr.
c     *  user input --                                             *   mixr.
c     *                                                            *   mixr.
c     *  card 1   --  units                                        *   mixr.
c     *     nout       output unit for mixed cross sections        *   mixr.
c     *     nin1       first input unit (endf or pendf)            *   mixr.
c     *     nin2       second input unit                           *   mixr.
c     *      ...        continue for nnin<=10 input units          *   mixr.
c     *                                                            *   mixr.
c     *  card 2   --  reaction list                                *   mixr.
c     *      mtn       list of nmt<=20 mt numbers for              *   mixr.
c     *                   the output reactions                     *   mixr.
c     *                                                            *   mixr.
c     *  card 3   --  material list                                *   mixr.
c     *     matn,      list of nmat<=10 pairs (matn,wtn) of mat    *   mixr.
c     *      wtn       numbers and associated weight factors       *   mixr.
c     *                                                            *   mixr.
c     *  card 4   --  temperature                                  *   mixr.
c     *     temp       temperature (use zero except for pendf tapes)*   mixr.
c     *                                                            *   mixr.
c     *  card 5   --  output material                              *   mixr.
c     *     matd       material number                             *   mixr.
c     *     za         za value                                    *   mixr.
c     *     awr        awr value                                   *   mixr.
c     *                                                            *   mixr.
c     *  card 6   --  file 1 comment card                          *   mixr.
c     *     des        description (60 char max)                   *   mixr.
```

❑ MIXR

```
mixr    / mixing the isotopic cross sections
 97 26 36 46 56       / nout, nin1 (endf or pendf), nin2
 203 204 205 206 207 301 444  / MTs for output
 2625 0.05845
 2631 0.91754
 2634 0.02119
 2637 0.00282            / MAT and weights pairs
 300.0                   / Temp
 2600 26000. 55.3670672  / output material: MAT, za, awr
 '26-Fe-  0 from ENDF/B-VII.1 '  / Description
```



NJOY modules

- **PURR**
  - Generates probability tables for treatment of URR self-shielding by Monte Carlo transport codes such as MCNP

```
purr / Process Unresolved Resonance Range if any
-21 -41 -26
9228 1 1 20 64/ matd ntemp nsigz nbin nladr
300.
1.E+10
0/
```

Infinite dilution for energy group g:

$$\sigma_{t(g)} = \frac{1}{E_2(g) - E_1(g)} \int_{E_1(g)}^{E_2(g)} \sigma(E)dE = \sum_{i=1}^{N} P_t(i,g)\sigma_t(i,g)$$

Table: Probability table (p_j, σ_j)

Prob. bins i / Group g	1	2	. . .	N (usually 15-20)
1	$P_t(1,1)$ $\sigma_t(1,1)$	$P_t(2,1)$ $\sigma_t(2,1)$		$P_t(N,1)$ $\sigma_t(N,1)$
2	$P_t(1,2)$ $\sigma_t(1,2)$	$P_t(2,2)$ $\sigma_t(2,2)$		$P_t(N,2)$ $\sigma_t(N,2)$
. . .				
M (< ladders)	$P_t(1,M)$ $\sigma_t(1,M)$	$P_t(2,M)$ $\sigma_t(2,M)$		$P_t(N,M)$ $\sigma_t(N,M)$

- UNRESR+ GROUPR generate group self-shielded data suitable for deterministic codes, but Bondarenko method is not useful for MC codes for which natural is probability tables method
- The **ladder method** generates pseudo resonance structures using random numbers based on the averaged resonance parameters.
- Probability tables for elastic scattering, capture and fission

NJOY modules

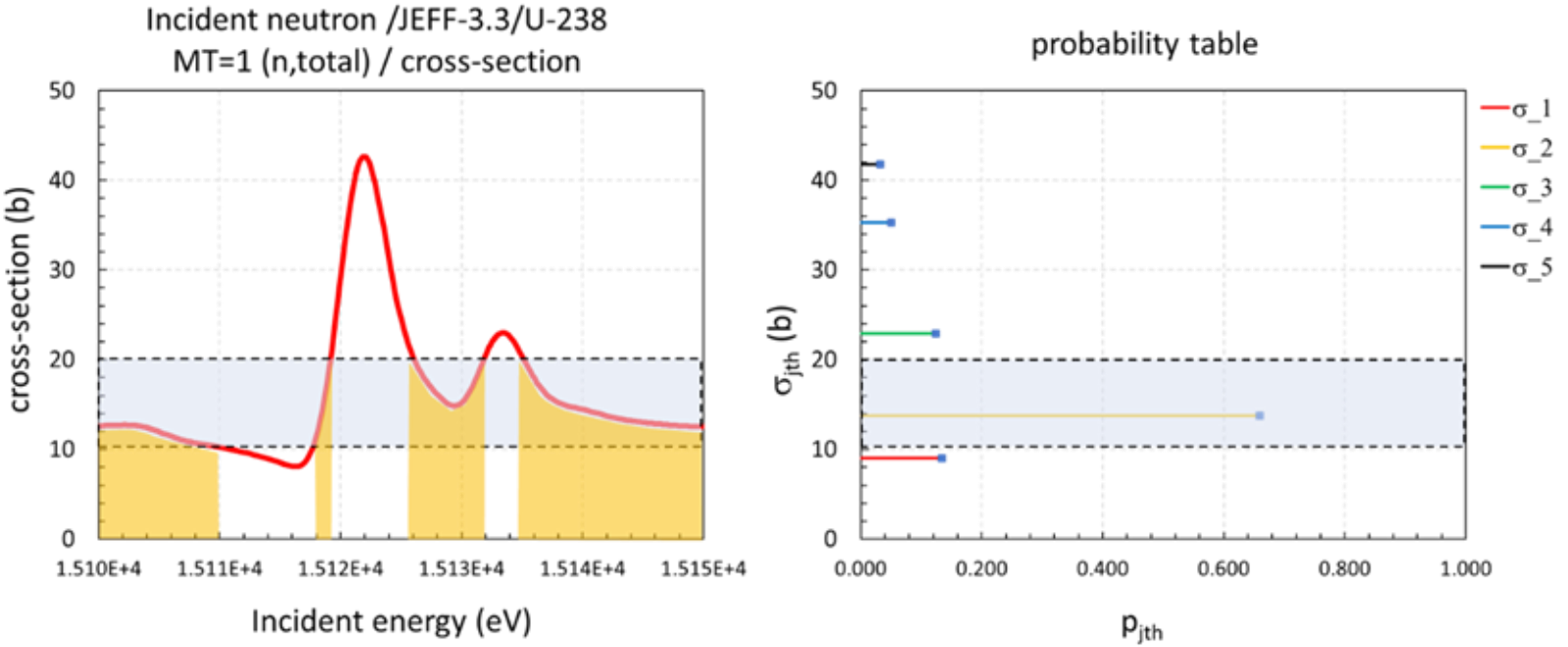
$$\bar{\sigma} = \frac{1}{(E_{max} - E_{min})} \int_{E_{min}}^{E_{max}} \sigma(E) dE = \frac{1}{(E_{max} - E_{min})} \sum_{i=1}^{M} \int_{E_{i-1}}^{E_i} \sigma(E) dE = \frac{1}{(E_{max} - E_{min})} \sum_{i=1}^{M} I_i$$

==

$$\bar{\sigma} = \int_{\sigma_{min}}^{\sigma_{max}} \sigma \cdot p(\sigma) d\sigma = \sum_{j=1}^{N} p_j \cdot \sigma_j$$

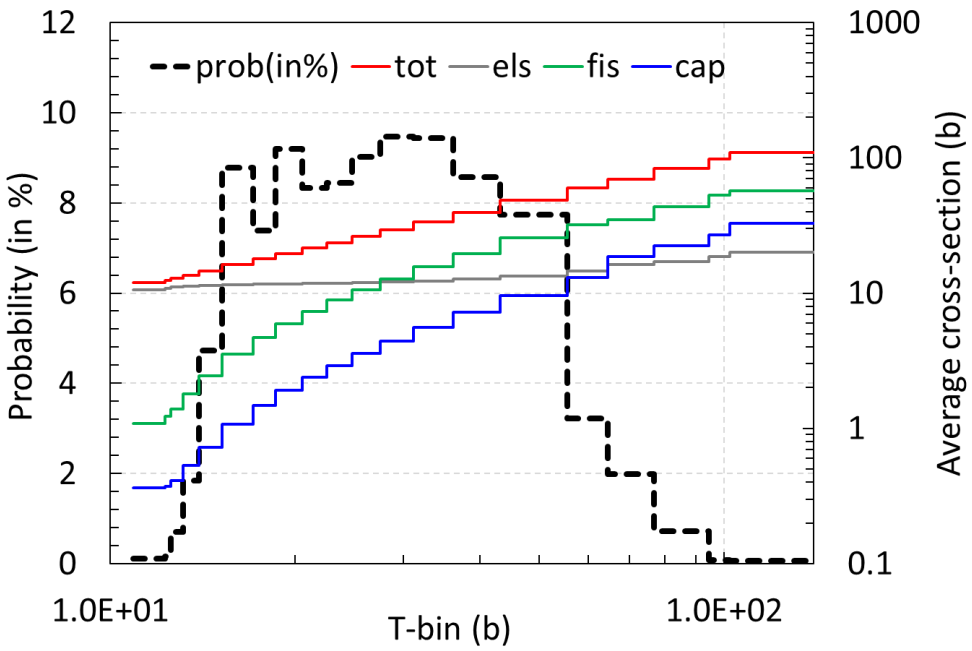
Figure. Scheme for ladder method: an example with 5-**ladders** and **5-bins**.

The dashed area corresponds to the band-3.



NJOY modules

Figure. An example of a probability table an average cross-section for ^{235}U from JENDL4.0 processed with NJOY2016.



NJOY options: Number of probability bins:20, number of resonance ladders: 64, incident energy 500 eV and temperature 300K.

- Procedure in Monte Carlo transport codes to use cross-section in the URR.

The MC code generates a random selection from the appropriate probability table as follows:

1) Select a uniform random number, 0<r<1 and then look up the conditional probability tables, setting $\sigma(E)=\sigma_j$ where $p_{j-1} < r < p_j$

2) All reaction cross-sections are selected from the same band, i.e with the same random number

NJOY modules

ACER

- Produces libraries in ACE format (A Compact ENDF) for MCNP general purpose Monte Carlo radiation transport code (and some other MC –based codes such as SERPENT, OpenMC)
- Advanced format compared to ENDF: provides random access by means of pointers to various data sets

```
acer / Prepare ACE files
-21 -26 0 27 28
1 0 1 .31/
'92-U-235 from JEFF3.1(JEFF3.1) NJOY 99.90 NEA Oct2005'/
9228 300.
1 1/
/
acer / Check ACE files
0 27 0 29 30
7 1 1 -1/
/
```

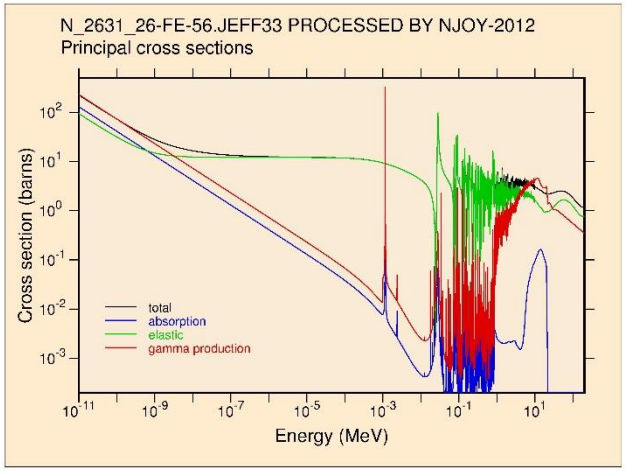
Suffix	ACE data class
c	Continuous energy neutron data
t	Thermal S(α,β) data
y	Dosimetry data
p	Photo-atomic data
u	Photonuclear data
h	Continuous-energy proton data
o	Continuous-energy deuteron data
r	Continuous-energy triton data
s	Continuous-energy He-3 data
a	Continuous-energy alpha data

NJOY modules

ACER + VIEWR

- Produces libraries in ACE format (A Compact ENDF) for MCNP general purpose Monte Carlo radiation transport code (and some other MC –based codes such as SERPENT, OpenMC)
- Advanced format compared to ENDF: provides random access by means of pointers to various data sets

```
acer                    / prepare ACE files
 -21 -26   0 27 28      /
  1   1   1   .95       /
 'n_2631_26-Fe-56.jeff33 processed by NJOY-2016' /
  2631 300              / MAT, Temp
 1 1                    /
 /
acer                    / check ACE files
  0   27   33   34 35   /
  7   1   1   -1        /
 /
viewr    / generation of .ps for all reactions
 33   43
```



NJOY modules

❑ ACER

For hydrogen bound in polyethylene

```
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .31/
'H-CH2   293.6 K from (JEFF3.1) NJOY99.90+NEA Oct2005'/
125 293.6 'poly01' /
 1001    0    0 /
 223 64 224  1  1 4.0 0/
```

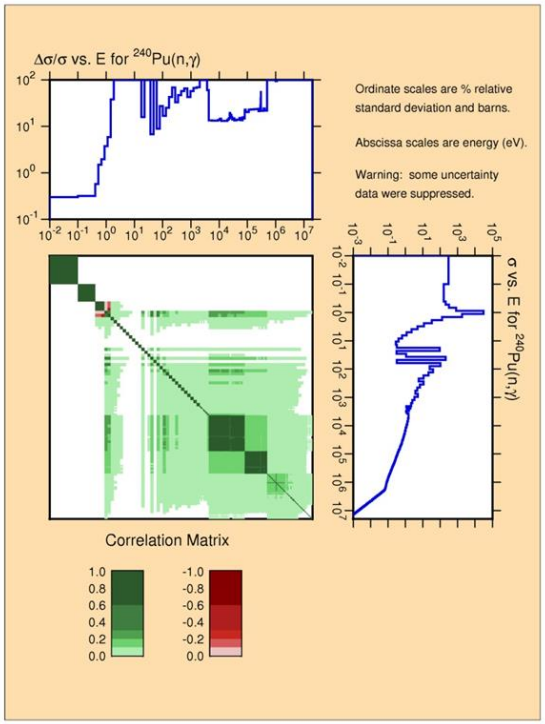
For hydrogen bound in water

```
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .31/
'H-H2O   293.6 K from (JEFF3.1) NJOY99.90+NEA Oct2005'/
125 293.6 'lwtr01' /
 1001    0    0 /
 222 64   0  0  1 4.0 0/
```

NJOY modules

ERRORR

- produces cross section and distribution covariances from error files in ENDF format
- converts energy dependent covariance information in ENDF format into multigroup form



ERRORR is able to process:

- MF31
- MF32/MF33
- MF34
- MF35
- MF40

```
moder
1 21
'moder for selected material'
20  9440
0/
reconr
21 24
'Pu240 PENDF from ENDF/B-VI.8'/
 9440 /
0.1 0.0 0.20 1.0e-8 9/
0/
broadr
21 24 25
 9440 1 0 1 0.
0.1 /
300.0
0/
errorr
21 25 0 27/
9440 17 2 1 1/
1 300.0 / mprint temp
0 33  /Procesa Lib 33 de incertidumbres
covr
27 57/
 3 1
'Pu240 from ENDF/B-VI.8'/
'Processing BOXER'/
9440 0 0 0 /
covr
27 0 37/
1
1.0E-5
1 1 0 1 1 / irelco(0=absol/1=relative)
9440 0 0 0 /
viewr
37 38/
stop
```

NJOY manual

- https://github.com/njoy/NJOY2016-manual/blob/master/njoy16.pdf

Available online at www.sciencedirect.com
ScienceDirect
ELSEVIER
Nuclear Data Sheets 111 (2010) 2739–2890
Nuclear D
Sheets
www.elsevier.com/loc

Methods for Processing ENDF/B-VII with NJOY

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(Received 2 July 2010; revised received 16 September 2010; accepted 1 October 2010)

The NJOY Nuclear Data Processing System is widely used to convert evaluations in the Evalu-

Example of available Processed Libraries

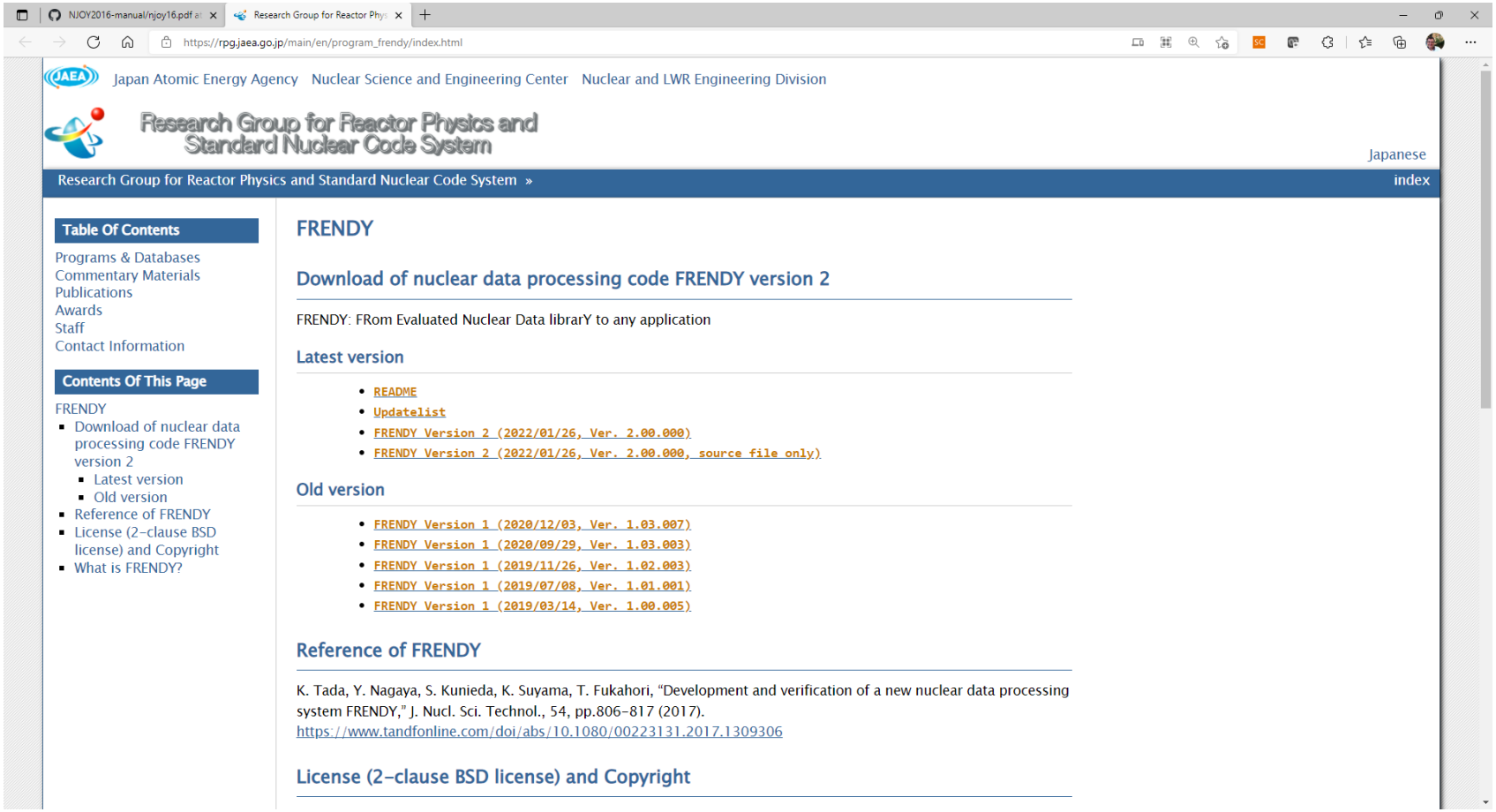
- MCJEFF3.1NEA, MCNP Neutron Cross Section Library based on JEFF3.1
  http://www.oecd-nea.org/tools/abstract/detail/nea-1768/
- MATJEFF31.BOLIB, JEFF-3.1 Multigr Coupled(199n + 42gamma) X-Section Lib.in MATXS Fmt for Nuclear Fission Applications
  http://www.oecd-nea.org/tools/abstract/detail/nea-1847/
- TSL-ACE/2013, Thermal Scattering Libraries processed to ACE format
  http://www.oecd-nea.org/tools/abstract/detail/nea-1883/

- WIMS-D (69 and 172 energy groups) , IAEA website
  https://www-nds.iaea.org/wimsd/
- ADS-2.0 Nuclear Data Library, Application Library for Accelerator Driven Systems and New Reactor Designs , IAEA website
  https://www-nds.iaea.org/ads/

- ACE - Library based on ENDF/B-VIII.0
  https://www.nndc.bnl.gov/endf-b8.0/

- ACE - Library based on JEFF-3.3
  https://www.oecd-nea.org/dbdata/jeff/jeff33/

FRENDY code



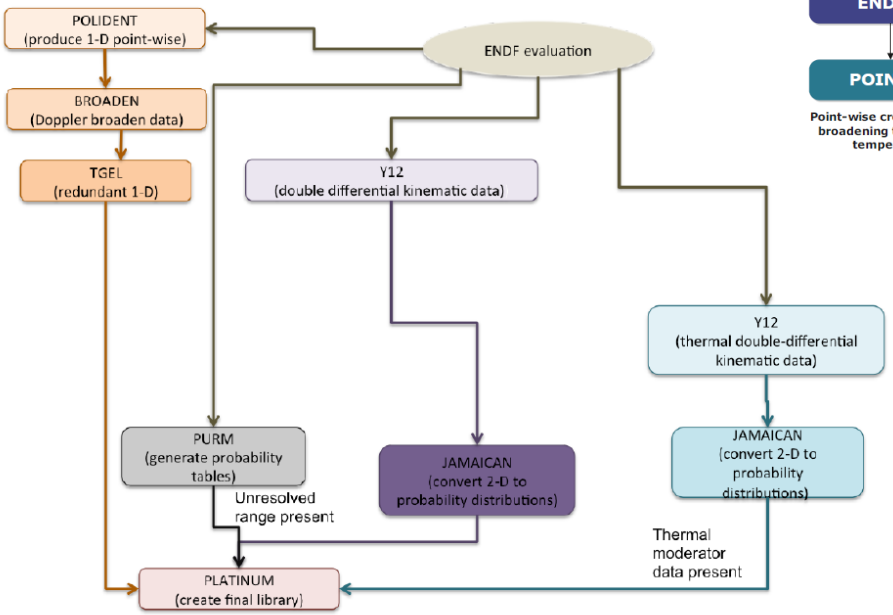
https://rpg.jaea.go.jp/main/en/program_frendy/index.html

AMPX System for SCALE codes

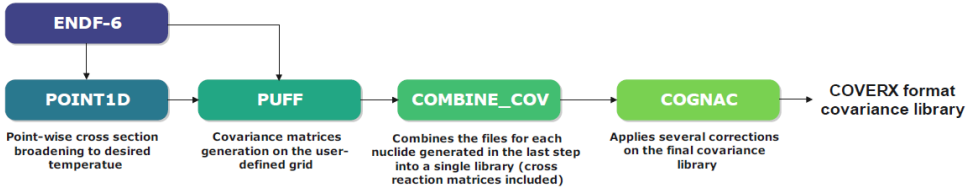
https://www.ornl.gov/onramp/ampx

https://www.ornl.gov/scale/scale/nuclear-data-fundamentals-and-ampx-libraries-generation-course

Processing of CE libraries with AMPX

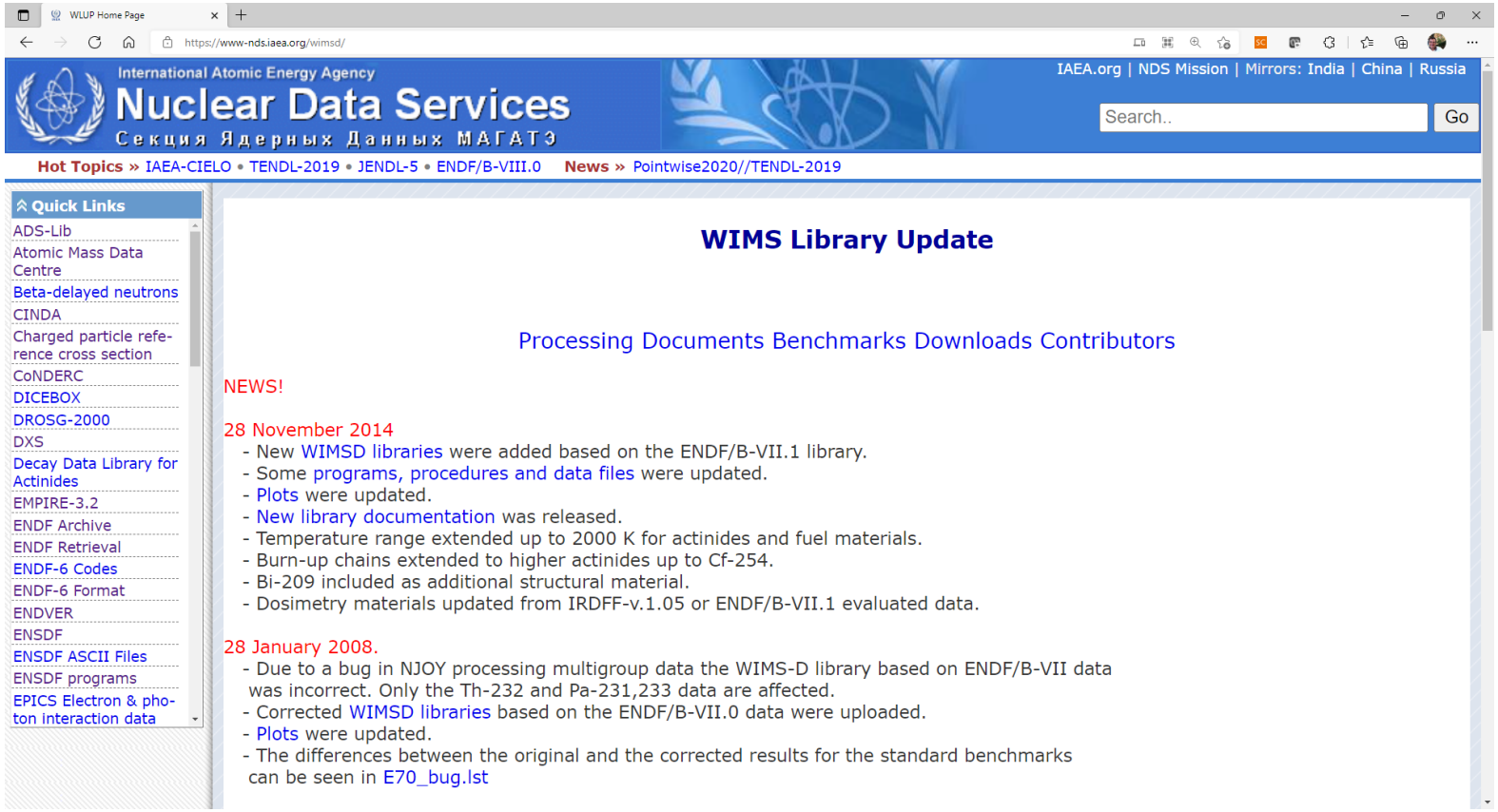


5. Processing of covariances with AMPX



Ref. A. Jiménez Carrascosa et al Processing of JEFF nuclear data libraries for the SCALE Code System, JEFDOC-2107, Nov 2021

Updating WIMSD Libraries



https://www-nds.iaea.org/wimsd/

IAEA activities in processing

https://www-nds.iaea.org/index-meeting-crp/TM-NDP-2021/

Special formats: HENDF to JANIS

- Processing into JANIS format : HENDF – Hybrid ENDF files

  - PENDF+MF2 (resonances)
  - BOXER
  - INTER

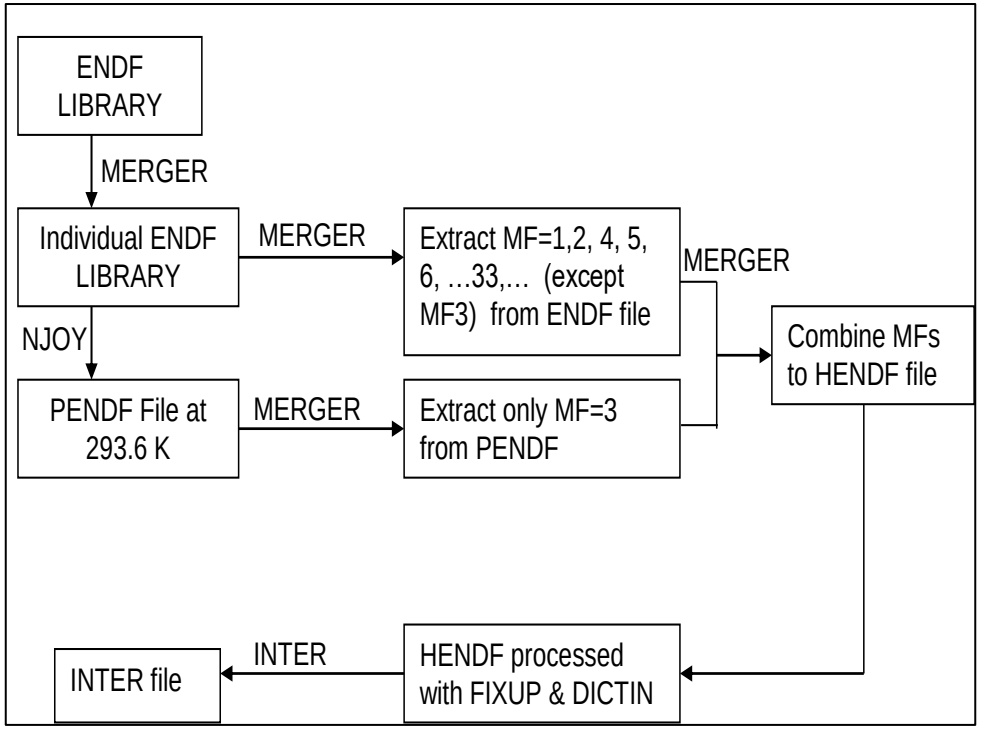
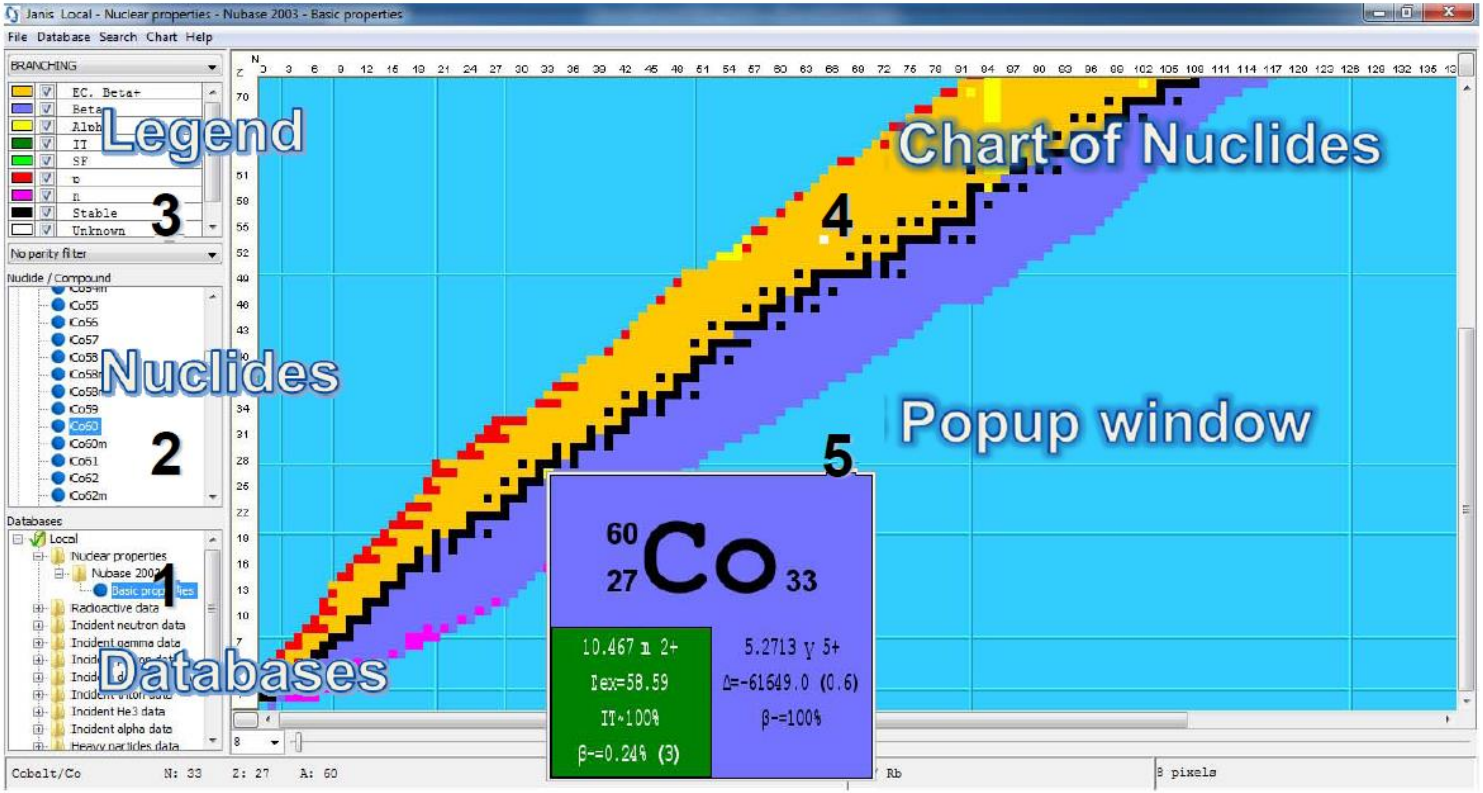


Figure. Flowchart of processing JANIS database from ENDF tapes

Basic visualization: JANIS Software

JAva-based **N**uclear Data **I**nformation **S**oftware designed to facilitate the visualisation and manipulation of nuclear data



http://www.oecd-nea.org/janis/

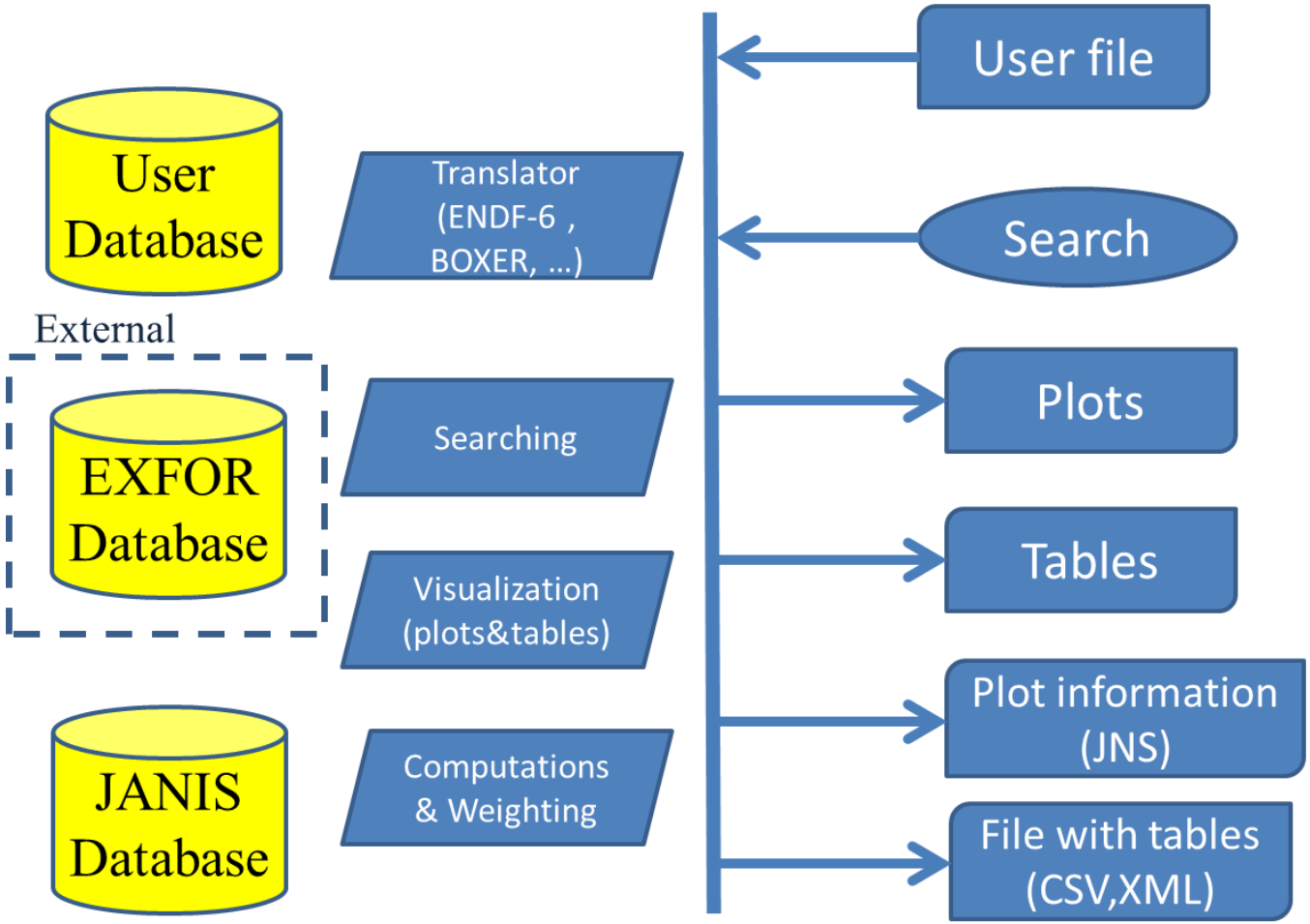
Basic visualization: JANIS Software

- Mainly a **graphical interface** giving access to:
  - Bibliographical nuclear reaction data (CINDA)
  - Experimental nuclear reaction data (EXFOR)
  - Evaluated nuclear reaction and decay data (e.g. JEFF, ENDF/B)
  - Basic properties of nuclei (NUBASE)

- Provides ways for:
  - **exploring** nuclear data libraries and databases
  - **visualisation** and **comparison** of data
  - **arithmetic operations**(normalisation, ratio, linear combination)
  - **some processing** (ratios, linear combinations, weighted average)

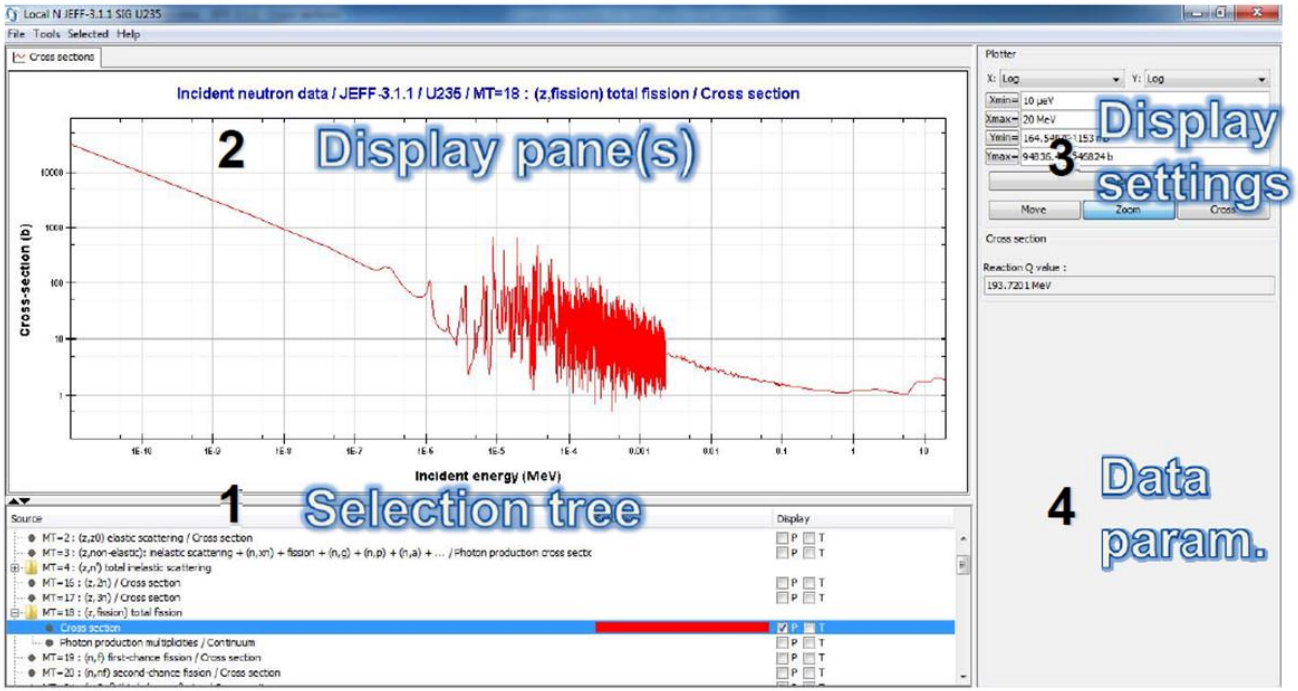
- Plots and numerical values can be **exported** in several formats:
  - PNG for images
  - WMF/EMF, PS, PDF for vectorial images
  - CSV, copy & paste to Excel for numerical values

Basic visualization: JANIS Software



Basic visualization: JANIS Software

- **JANIS – Plot (renderer) window**



1- Selection tree: To select the data you want to display

2- Display panes: To display textual information, tabulated values, plots, decay paths

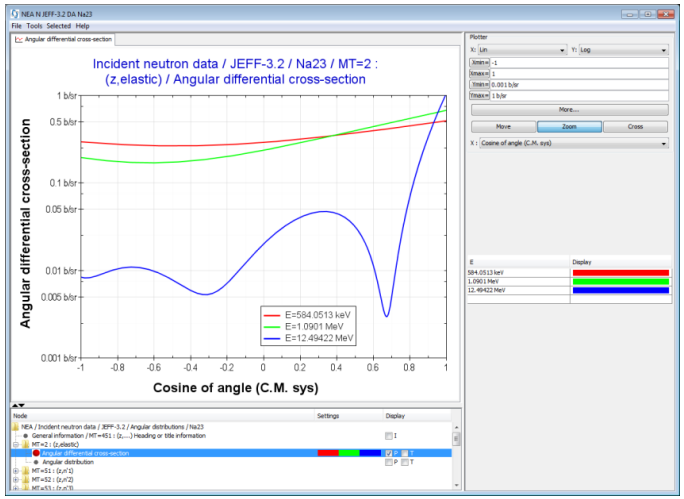
3- Display pane (plot) settings: To adjust the settings of the plot or table

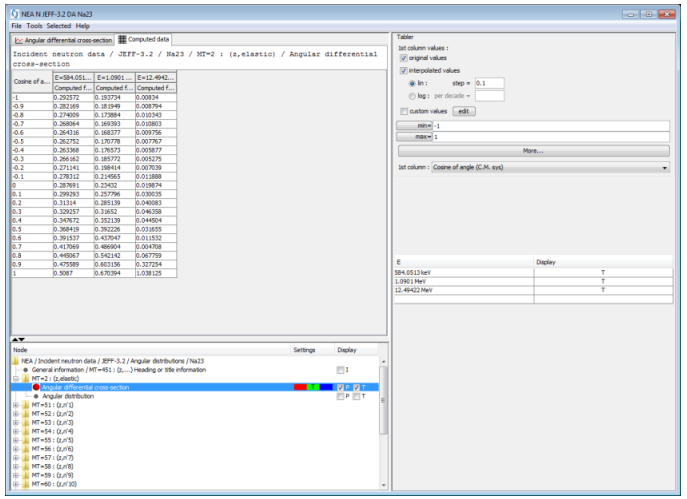
4- Data parameters: To display additional information on the selected data, and select variable values for distributions, yields..

Basic visualization: JANIS Software

- **Others panels**
  - Text panels
  - Decay paths
  - Color maps

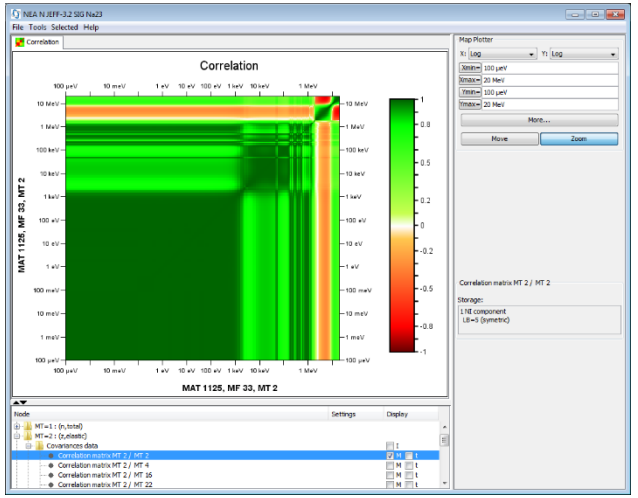
- **Save/Export**
  - JNS File to open
  - Figures in PNG or PS





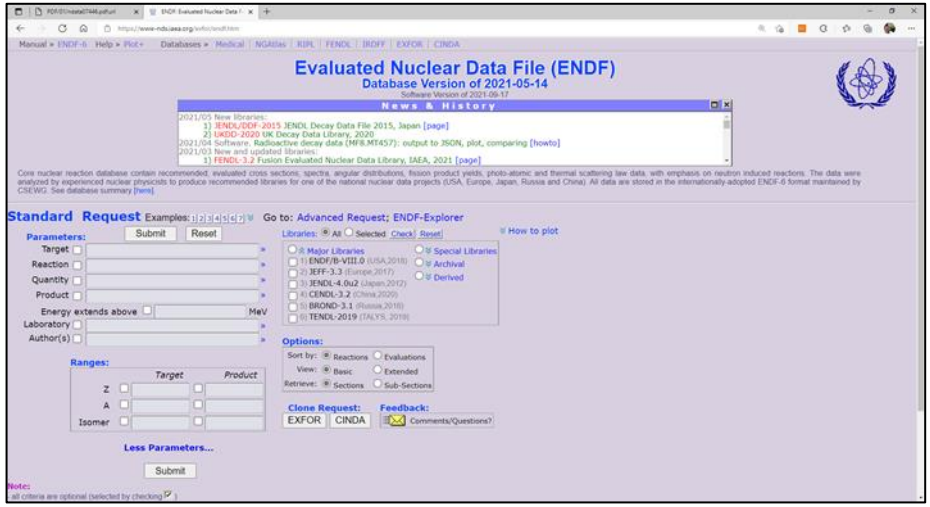
- **Run command line**

```
C:\java -jar janis.jar -o XX.png -render XX.jns png 1024 768
```

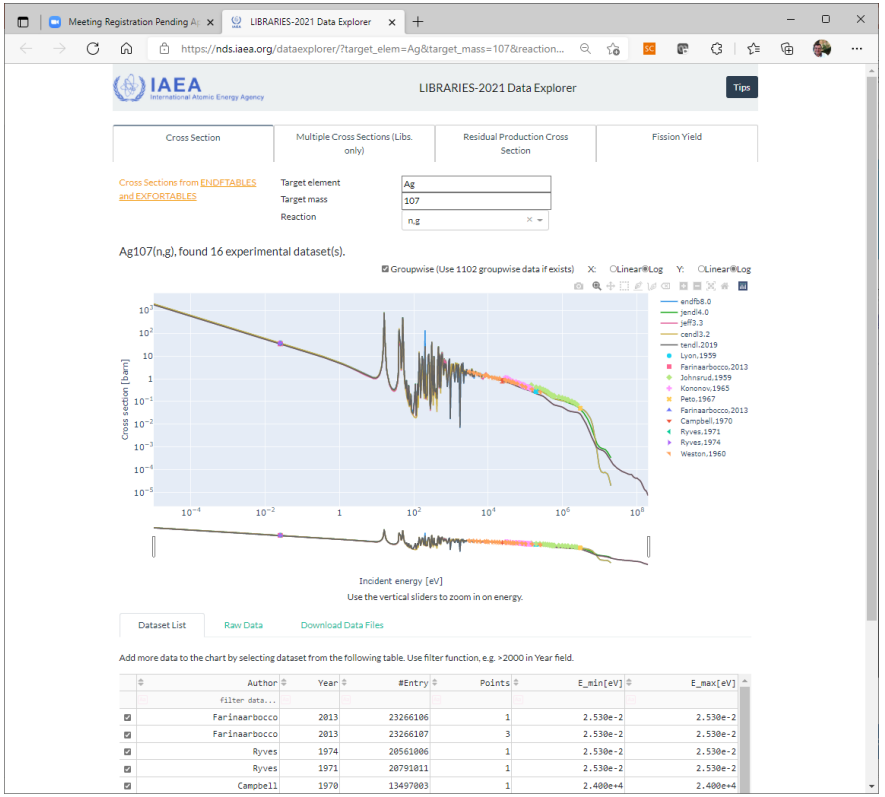


Visualization: Other tools

Figure. The IAEA/NDS retrieval system's website



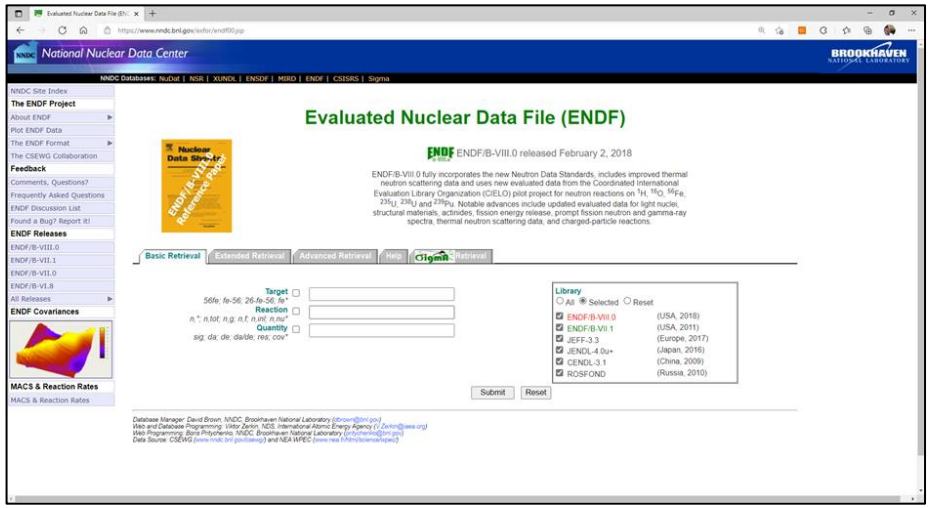
https://www-nds.iaea.org/exfor/endf.htm



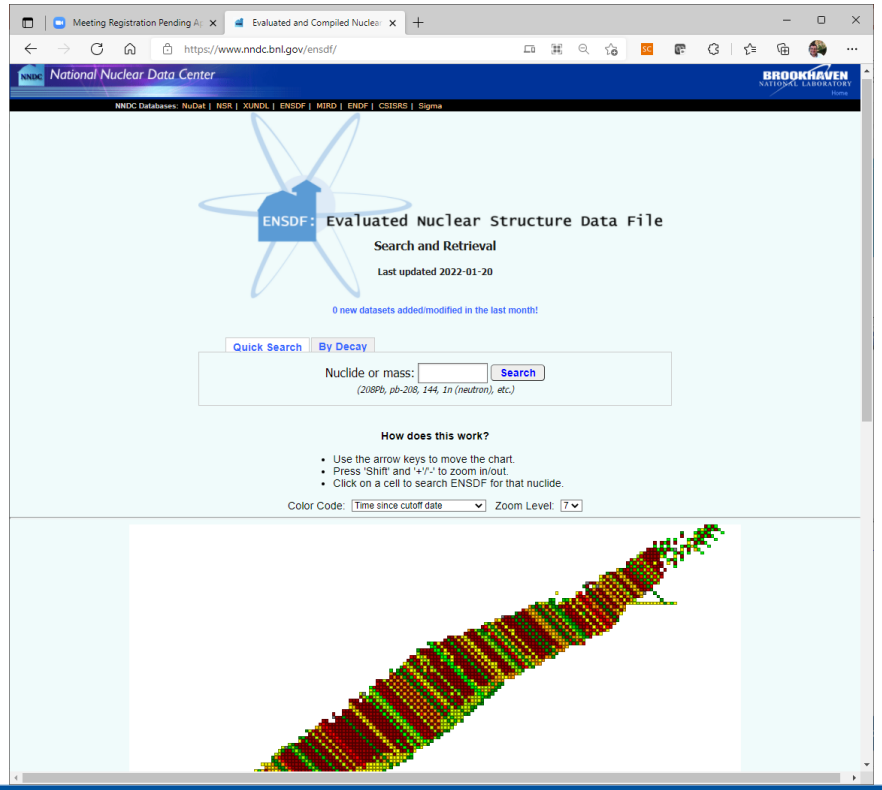
https://nds.iaea.org/dataexplorer

Visualization: Other tools

Figure. The NNDC retrieval system's website



https://www.nndc.bnl.gov/exfor/endf00.jsp



https://www.nndc.bnl.gov/ensdf/

Conclusion

- *Monte Carlo simulation codes and necessary data*
- *Deterministic codes and necessary data*
- *Processing of nuclear data: tools and output formats*
- *Steps in the nuclear data library processing for generations of processed nuclear data libraries: resonances. Doppler broadening, treatment of unresolved resonance region, …*
- *Basic visualization*