

# *Simulation codes and data processing tools*

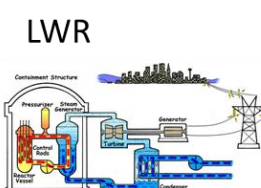
**O. Cabellos**

*Universidad Politécnica de Madrid (UPM), Madrid, Spain*

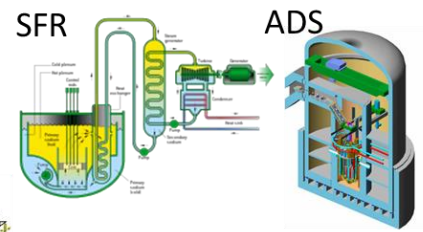
E-mail: [oscar.cabellos@upm.es](mailto:oscar.cabellos@upm.es)

- ❑ *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



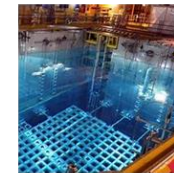
**LWR**



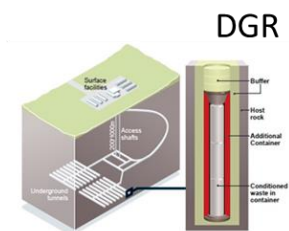
**SFR**      **ADS**



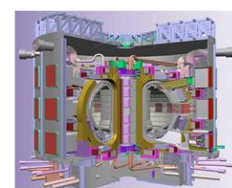
**SMRs**



**Spent Fuel**




**DGR**



**Fusion/ITER**

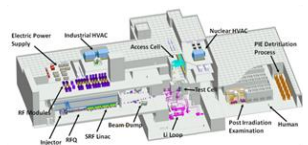
**Nuclear Data for Applications** (fission and fusion, radiation protection, nuclear medicine, nuclear security, object and materials analysis,... )  
**and Science** (reactions and structure of nuclei, astrophysics, basic physics,...)



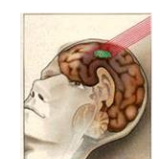
**Neutrino's physics**



**Space technology**



**IFMIF/DONES**



**Medical applications**



**Astrophysics**

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

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

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

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

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

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

Doppler ignored

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

$$\Sigma_s = \int dE' d\Omega' \Sigma_{s(E \rightarrow E', \Omega \rightarrow \Omega')}$$

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

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

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

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

- 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 ...

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

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

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

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

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

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

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

Doppler ignored

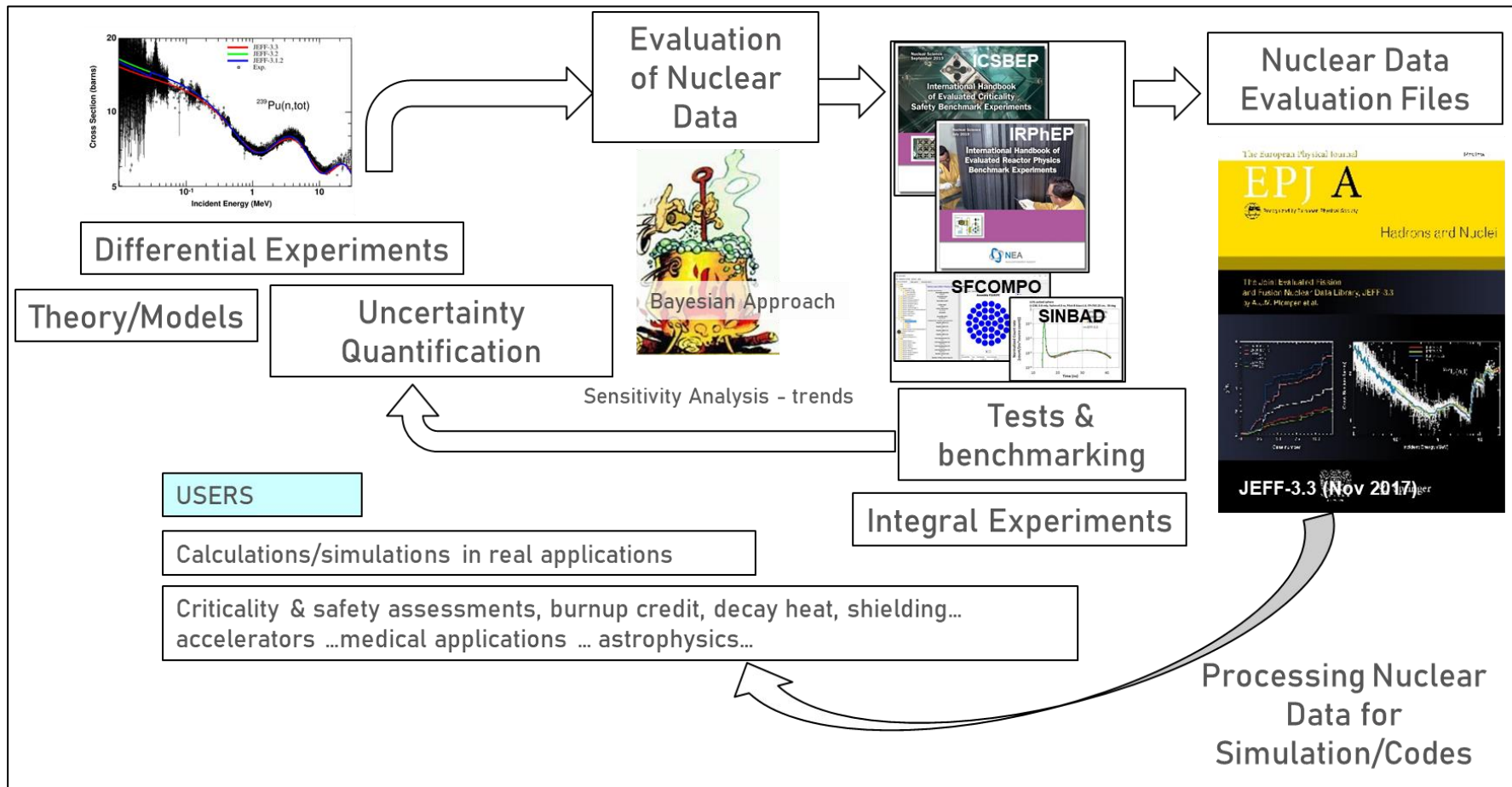
$$\Sigma_T = \Sigma_a + \Sigma_s$$

$$\Sigma_s = \int dE' d\Omega' \Sigma_{s(E \rightarrow E', \Omega \rightarrow \Omega')}$$

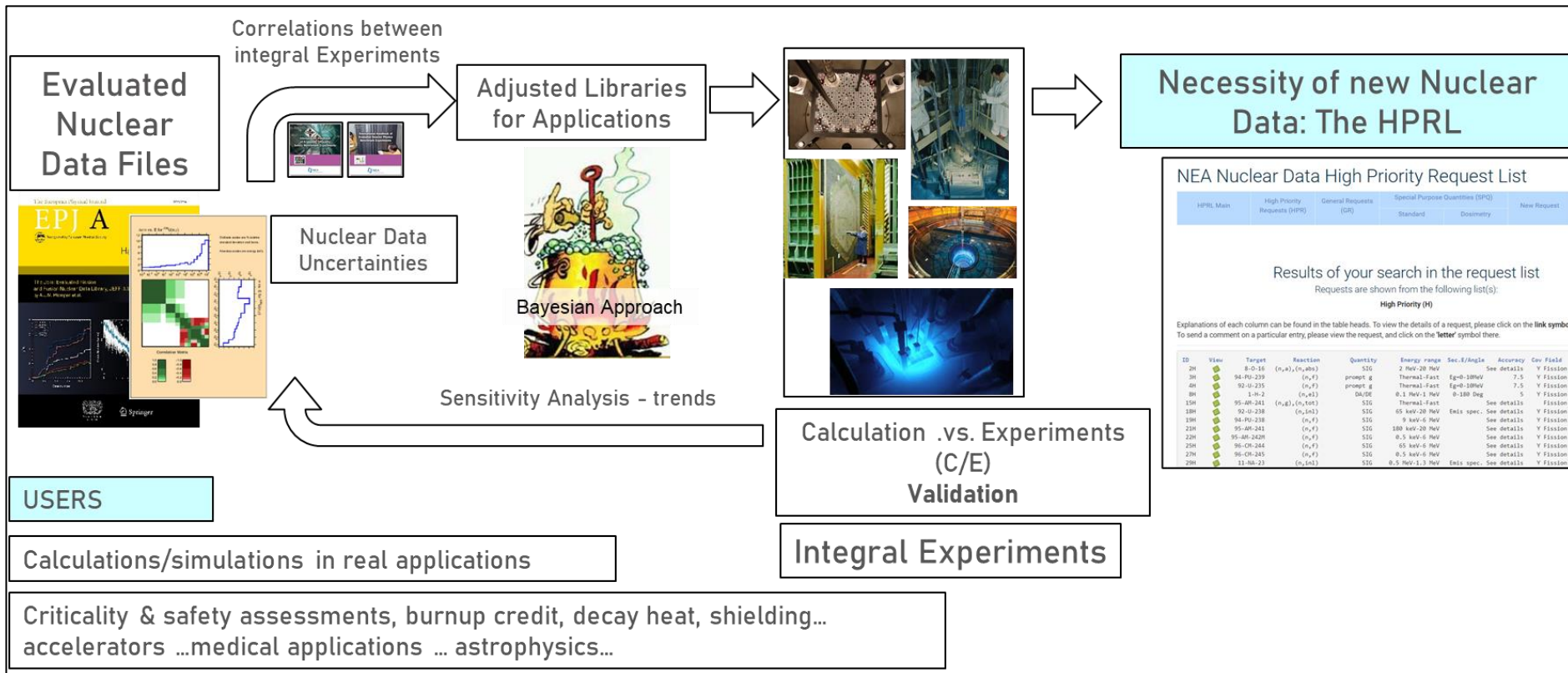
- Activation codes: FISPACT, ORIGEN, ACAB, DARWIN, ...

- Burnup/Depletion codes: EVOLCODE, VESTA, CASMO, SERPENT, ...

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

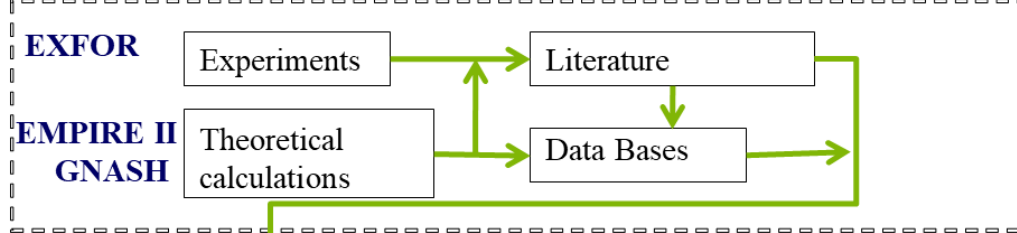


❑ The End-Users are the bridge between the applications and the necessity of new nuclear data

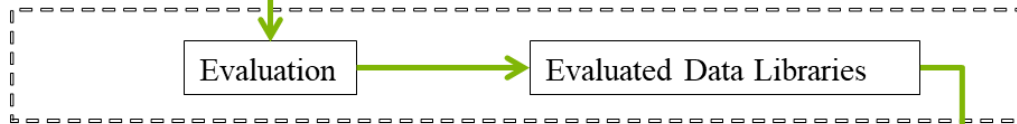


## □ Activities associated with Nuclear Data

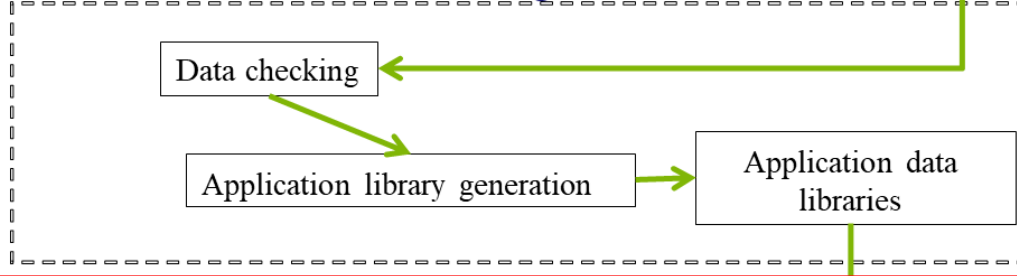
### 1. Basic Nuclear data Production



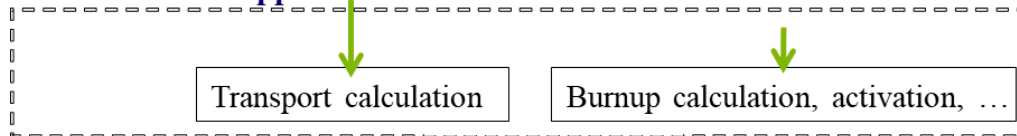
### 2. Nuclear Data Evaluation



### 3. Evaluated Nuclear Data "Processing"



### 4. Nuclear Data Applications



#### Processing Codes:

NJOY  
CALENDF  
PREPRO  
AMPX, PUFF  
FRENDY, ACEMAKER, ...

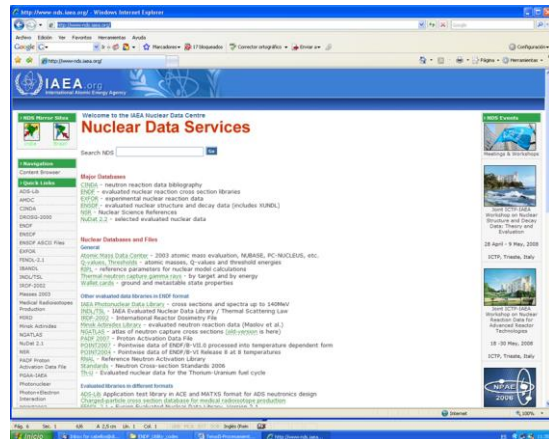
Ref: A.Trkov. "Status and Perspective of Nuclear Data Production, Evaluation and Validation". Nuclear Engineering and technology, Vol.37 No.1 (2005)



- ENDF Utility codes for checking data formats and internal consistency developed at NNDC in Brookhaven  
<https://www.nndc.bnl.gov/endl/>
- ENDF Pre-Processing codes of the IAEA: PREPRO2021  
<http://www-nds.iaea.org/ndspub/endl/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/endl/endver/>
- JANIS package + JANIS handbook  
[https://www.oecd-nea.org/jcms/pl\\_39910/janis](https://www.oecd-nea.org/jcms/pl_39910/janis)  
[https://www.oecd-nea.org/jcms/pl\\_44624/janis-books](https://www.oecd-nea.org/jcms/pl_44624/janis-books)

## Brief Description

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



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

<http://www-nds.iaea.org/ndspub/endl/utility/index.html>

**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

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

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

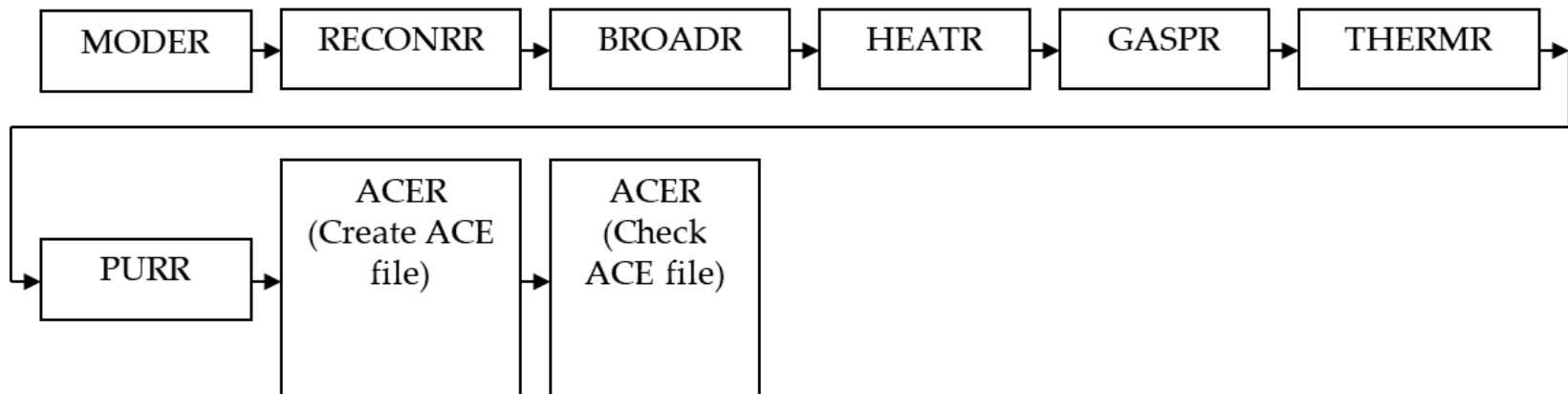
$$G = \frac{2}{\sqrt{\pi}} \frac{I}{\sigma(kT)}$$

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

<http://www-nds.iaea.org/ndspub/endl/prepro>

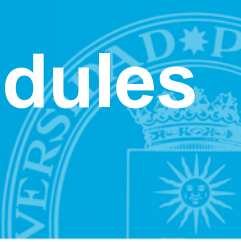
- NJOY is a comprehensive system for generating application libraries, developed at Los Alamos National Laboratory.

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



<https://github.com/njoy/NJOY2016>

<https://github.com/njoy/NJOY21>



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

## ❑ MODER

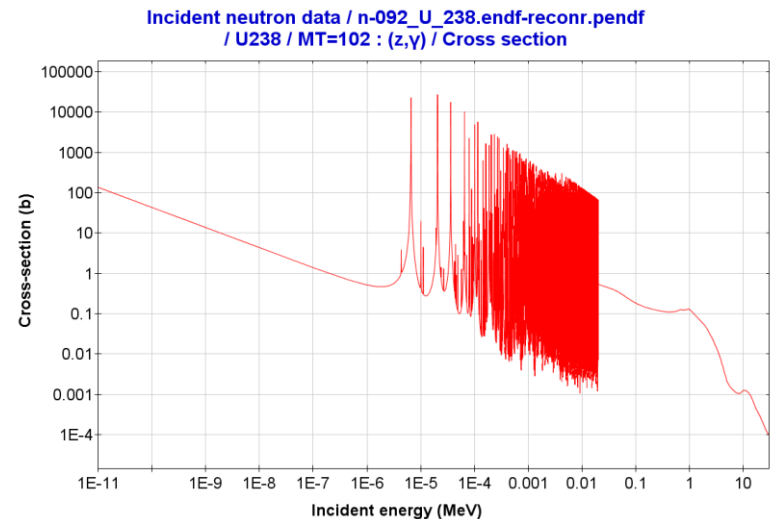
- Copy a tape from ascii/binary format to binary/ascii
- Extract an individual material from a multi-material tape and copy (including ascii/binary or binary/ascii conversion) to a new tape
- Create a custom multi-material tape (including ascii/binary or binary/ascii conversion)
- Strongly recommend 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/
```

## □ 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/
```



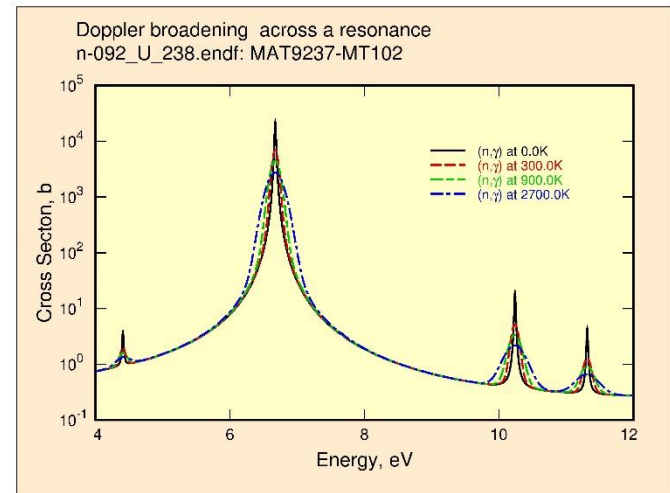
## ❑ BROADR

### ○ 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
  
```





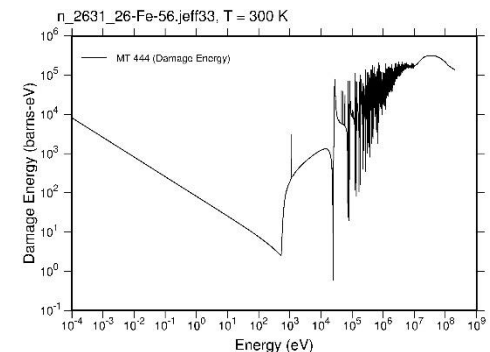
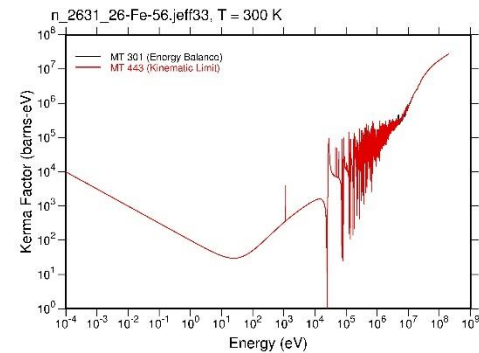
## ☐ HEATR: Total Heating, Heating by Reaction, Radiation Damage

- 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



## □ 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)

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

$\varphi_0$  is scalar flux,  $E^*$  is the effective energy in  $[E_1, E_2]$  where cross sections are slowly varying with  $E$

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

$\varphi_1$  is  $P_1$  component of neutron flux proportional to neutron current

Shape of flux:

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

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

## GROUPR

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

```
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/
```

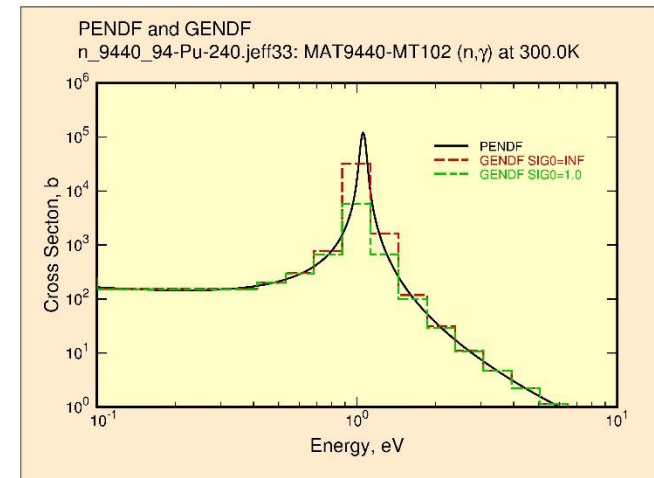
Table: Standard neutron group structures

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-ii-a 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

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



## ❑ THERMR

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

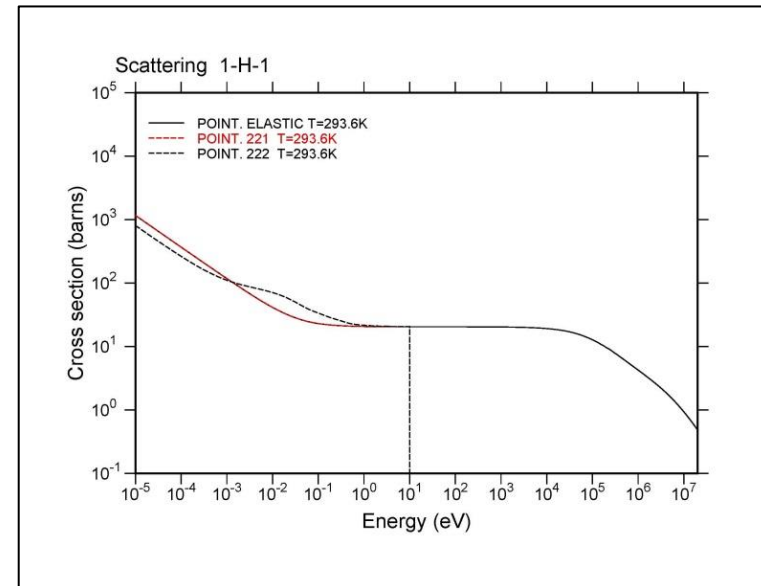
```

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 <sub>2</sub> )	37	223	iel	free C
H(liquidCH <sub>4</sub> )	33			
H(solidCH <sub>4</sub> )	34			
C <sub>6</sub> H <sub>6</sub>	40	227		none
D(D <sub>2</sub> O)	11	228		free O
D(paraD <sub>2</sub> )	12			
D(orthoD <sub>2</sub> )	13			
H(H <sub>2</sub> O)	1	222		free O
H(paraH <sub>2</sub> )	2			
H(orthoH <sub>2</sub> )	3			
Zr(ZrH <sub>n</sub> )	58	235,236	iel	
H(ZrH <sub>n</sub> )	7	225,226	iel	
U(UO <sub>2</sub> )	76	241,242	coh	
O(UO <sub>2</sub> )	75	239,240	coh	



## □ MIXR

```

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

```

```

* mixr.
* mixr.
* mixr.
* mixr.
* mixr.
* mixr.
* mixr.
* mixr.
* mixr.
* mixr.
* mixr.

```

```

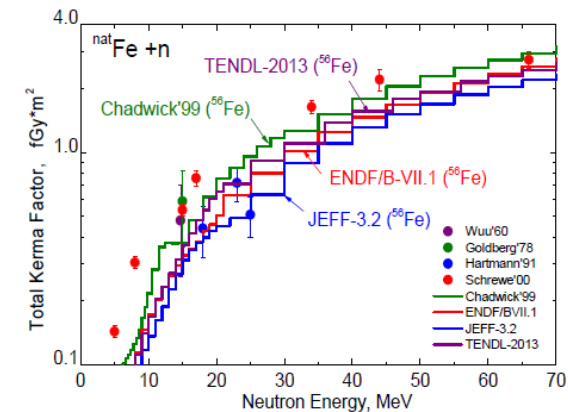
mixr / mixing the isotopic cross sections
97 26 36 46 56 / nout, nin1 (endf or pendf), nin2
203 204 205 206 207 301 444 / MTs for output
2625 0.05845
2631 0.91754
2634 0.02119
2637 0.00282 / MAT and weights pairs
300.0 / Temp
2600 26000. 55.3670672 / output material: MAT, za, awr
'26-Fe- 0 from ENDF/B-VII.1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

```

```

* mixr.
* mixr.
* mixr.
* mixr.
* mixr.
* mixr.
* mixr.
* mixr.
* mixr.
* mixr.
* mixr.

```



## □ 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 ( $p_j, \sigma_j$ )**

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

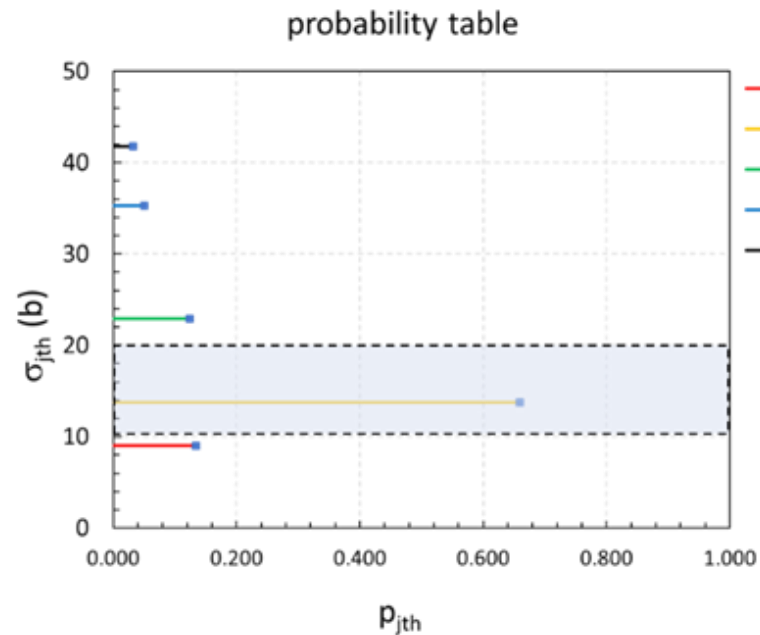
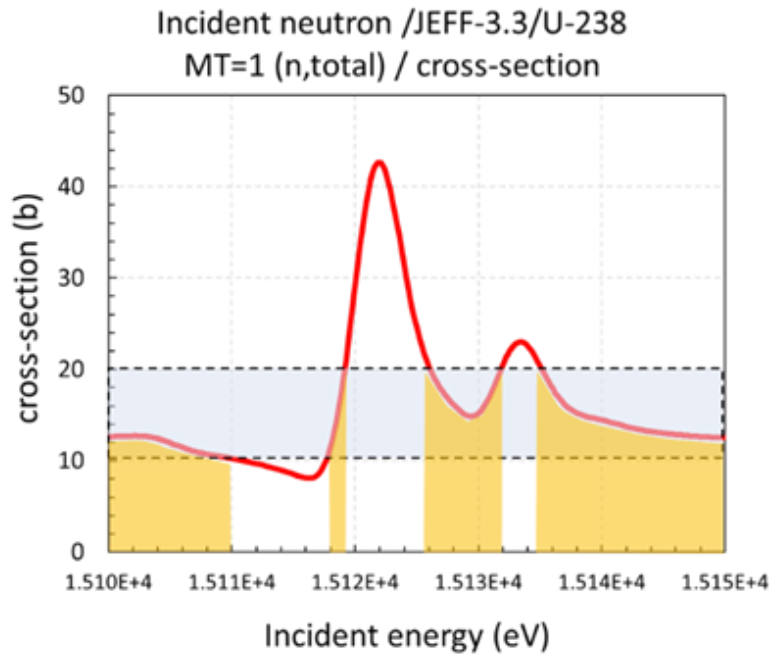
- UNRESR+ GROUPT generate group self-shielded data suitable for deterministic codes, but Bondarenko method is not useful for MC codes for which natural is probability tables method

- The **ladder method** generates pseudo resonance structures using random numbers based on the averaged resonance parameters.
- Probability tables for elastic scattering, capture and fission

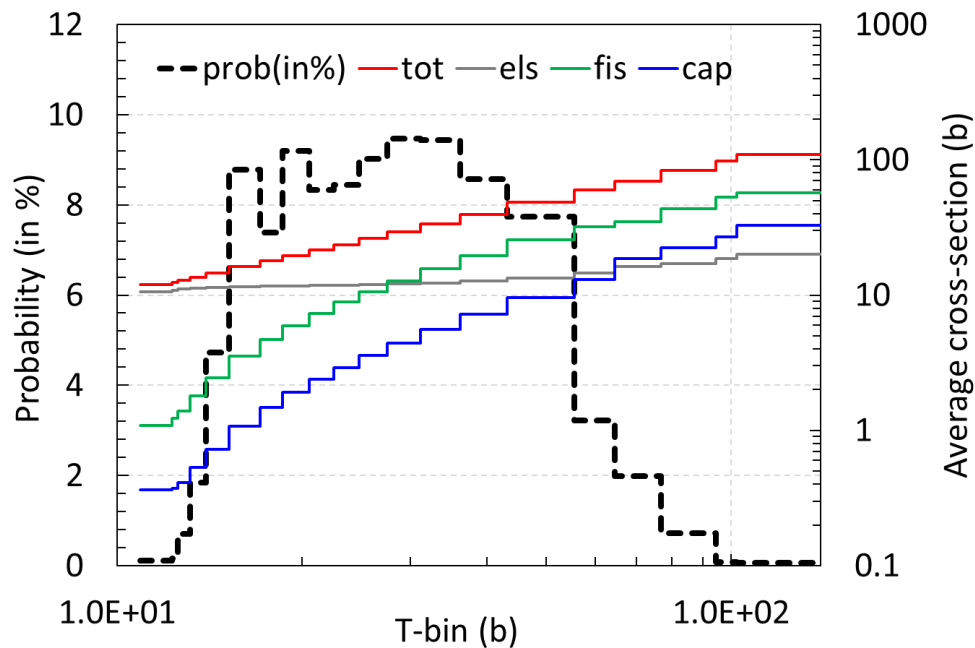
$$\bar{\sigma} = \frac{1}{(E_{max} - E_{min})} \int_{E_{min}}^{E_{max}} \sigma(E) dE = \frac{1}{(E_{max} - E_{min})} \sum_{i=1}^M \int_{E_{i-1}}^{E_i} \sigma(E) dE = \frac{1}{(E_{max} - E_{min})} \sum_{i=1}^M I_i \quad == \quad \bar{\sigma} = \int_{\sigma_{min}}^{\sigma_{max}} \sigma \cdot p(\sigma) d\sigma = \sum_{j=1}^N p_j \cdot \sigma_j$$

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

The dashed area corresponds to the [band-3](#).



**Figure.** An example of a probability table and average cross-section for  $^{235}\text{U}$  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



## ❑ 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/
/
```

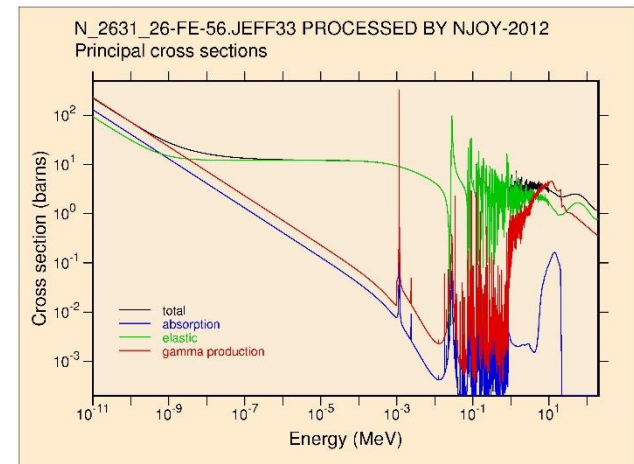
Suffix	ACE data class
c	Continuous energy neutron data
t	Thermal S( $\alpha,\beta$ ) data
y	Dosimetry data
p	Photo-atomic data
u	Photonuclear data
h	Continuous-energy proton data
o	Continuous-energy deuteron data
r	Continuous-energy triton data
s	Continuous-energy He-3 data
a	Continuous-energy alpha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

## ❑ 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
  
```



## ❑ ACER

For hydrogen bound in polyethylene

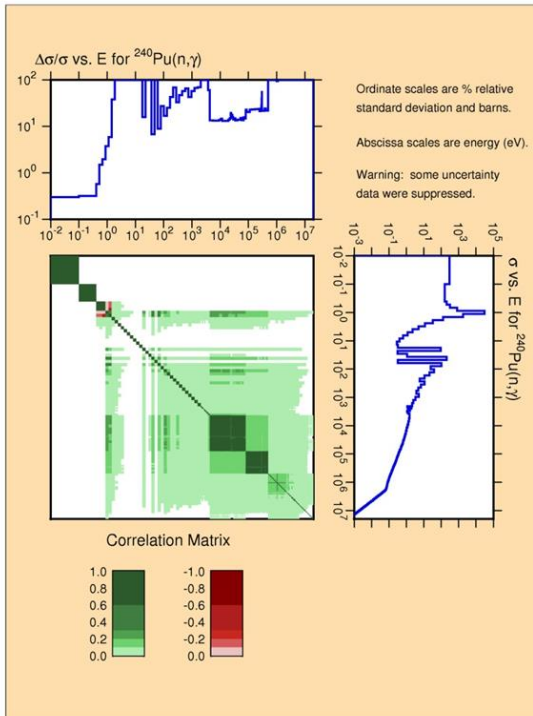
```
acer / Prepare ACE files
-21 -27 0 28 29
2 0 1 .31/
'H-CH2 293.6 K from (JEFF3.1) NJOY99.90+NEA Oct2005'/
125 293.6 'poly01' /
1001 0 0 /
223 64 224 1 1 4.0 0/
```

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/
```

## ❑ 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
  
```

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



ELSEVIER

Available online at [www.sciencedirect.com](http://www.sciencedirect.com)



ScienceDirect

Nuclear Data Sheets 111 (2010) 2739–2890

[www.elsevier.com/loc](http://www.elsevier.com/loc)

**Nuclear Data Sheets**

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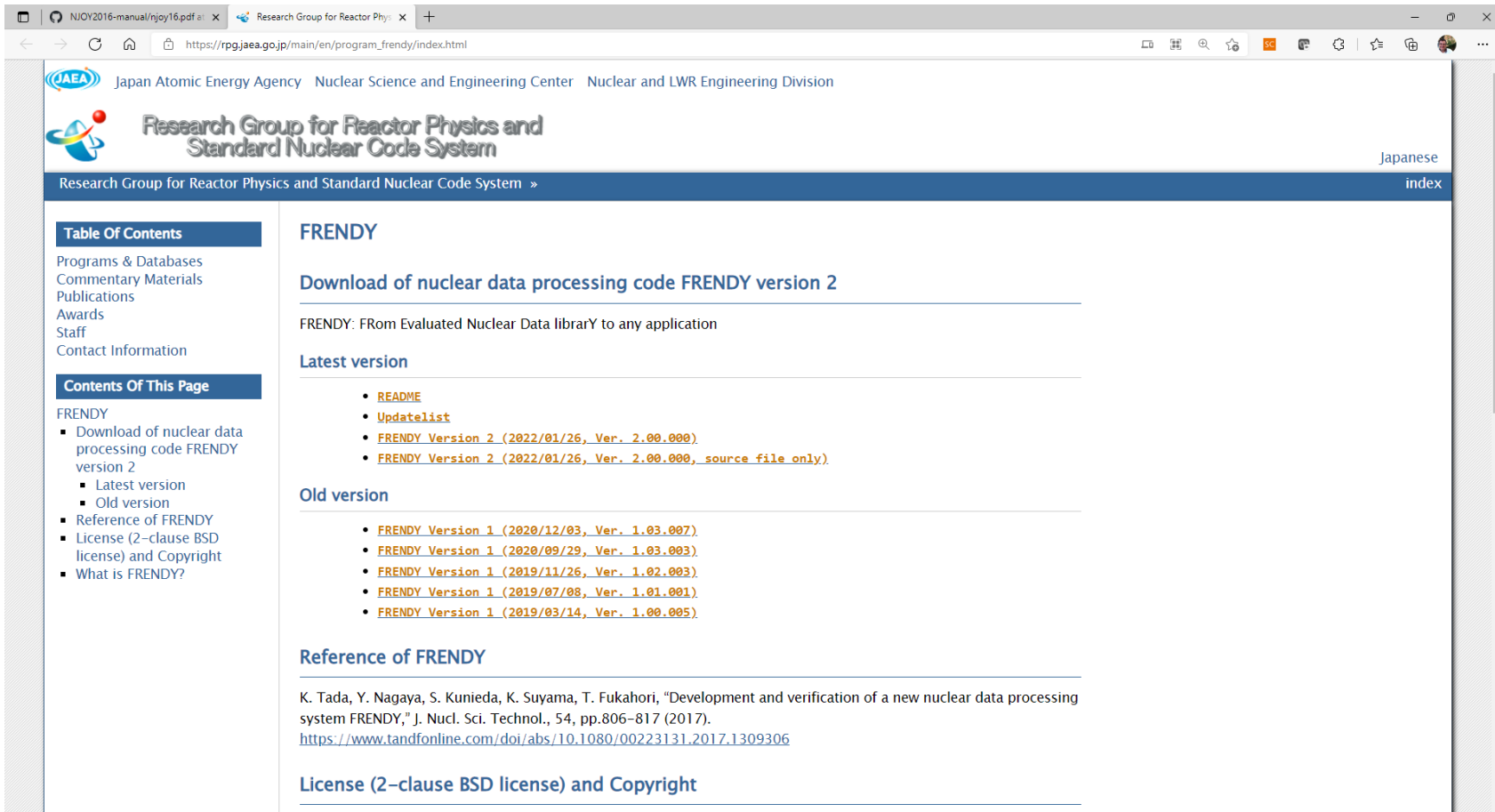
## Methods for Processing ENDF/B-VII with NJOY

R. E. MacFarlane\* and A. C. Kahler†  
*Nuclear and Particle Physics, Astrophysics and Cosmology  
Theoretical Division  
Los Alamos National Laboratory,  
Los Alamos, NM 87545*

(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 Evalua...

- 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/endl-b8.0/>
- ACE - Library based on JEFF-3.3  
<https://www.oecd-nea.org/dbdata/jeff/jeff33/>



The screenshot shows a web browser displaying the homepage of the Research Group for Reactor Physics and Standard Nuclear Code System. The page is in English and features a navigation menu on the left with sections for 'Table Of Contents' and 'Contents Of This Page'. The main content area is titled 'FRENDY' and includes a 'Download of nuclear data processing code FRENDY version 2' section. Below this, there are links for 'Latest version' and 'Old version', each with a list of specific releases. A 'Reference of FRENDY' section provides a citation for a paper by K. Tada et al. (2017). The 'License (2-clause BSD license) and Copyright' section is also visible at the bottom of the main content area.

Japan Atomic Energy Agency Nuclear Science and Engineering Center Nuclear and LWR Engineering Division

Research Group for Reactor Physics and Standard Nuclear Code System

Japanese index

Research Group for Reactor Physics and Standard Nuclear Code System »

## Table Of Contents

- Programs & Databases
- Commentary Materials
- Publications
- Awards
- Staff
- Contact Information

## Contents Of This Page

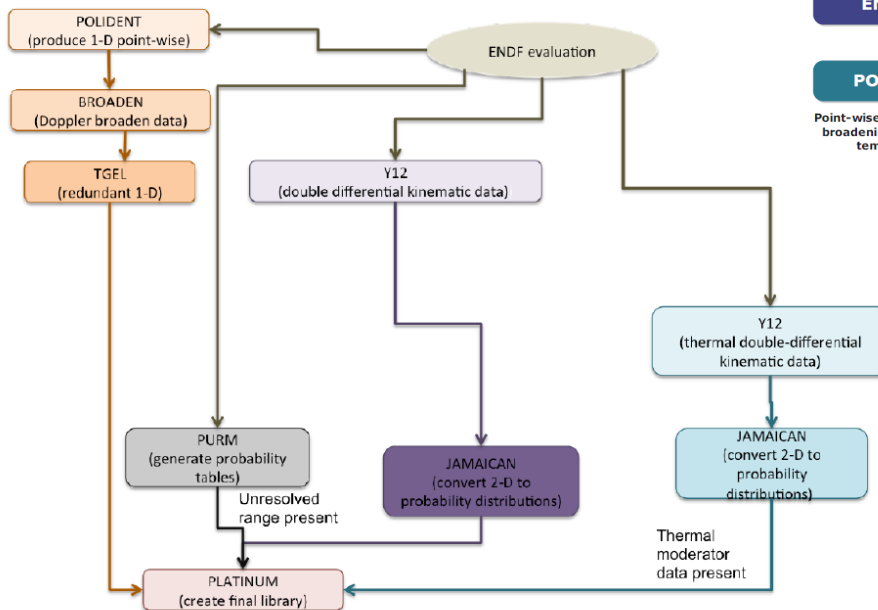
- FRENDY
  - Download of nuclear data processing code FRENDY version 2
    - Latest version
    - Old version
  - Reference of FRENDY
  - License (2-clause BSD license) and Copyright
  - What is FRENDY?

[https://rpg.jaea.go.jp/main/en/program\\_frendy/index.html](https://rpg.jaea.go.jp/main/en/program_frendy/index.html)

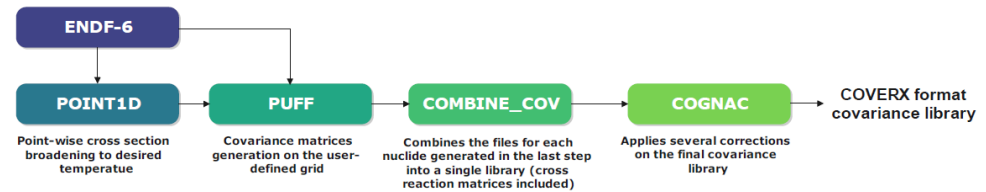
<https://www.ornl.gov/onramp/ampx>

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

## Processing of CE libraries with AMPX

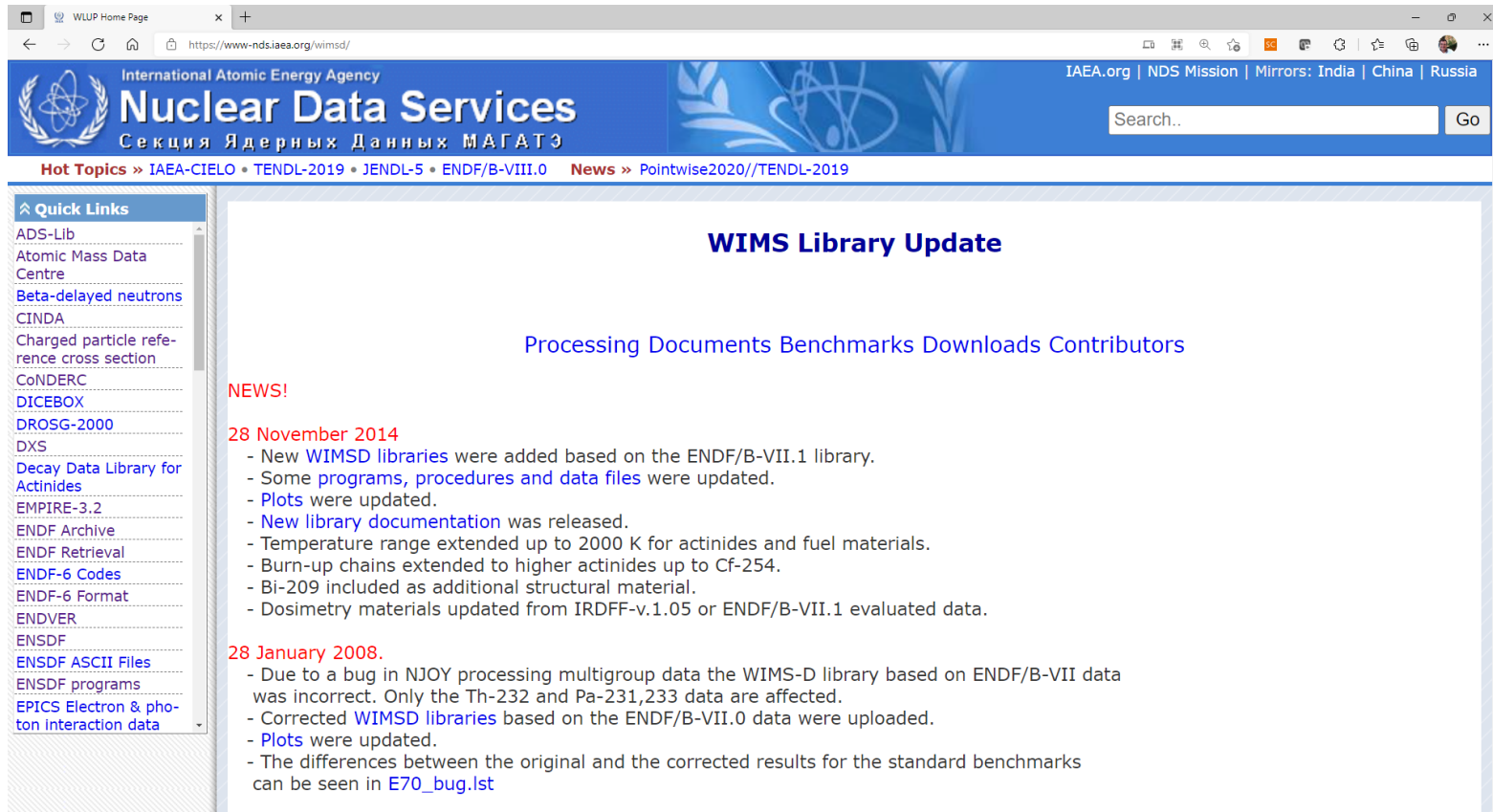


## 5. Processing of covariances with AMPX



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





The screenshot shows the WIMSD website interface. At the top, there is a navigation bar with the IAEA logo and text: "International Atomic Energy Agency Nuclear Data Services Секция Ядерных Данных МАГАТЭ". To the right of the navigation bar is a search box with the text "Search.." and a "Go" button. Below the navigation bar, there are "Hot Topics" and "News" links. The main content area is titled "WIMS Library Update" and contains a sub-header "Processing Documents Benchmarks Downloads Contributors". Underneath, there is a "NEWS!" section with two entries: "28 November 2014" and "28 January 2008". Each entry lists several updates to the WIMSD libraries, including new additions, updated programs and data files, and corrections to existing data. A left sidebar contains a "Quick Links" menu with various links to different data services and archives.

International Atomic Energy Agency  
**Nuclear Data Services**  
Секция Ядерных Данных МАГАТЭ

IAEA.org | NDS Mission | Mirrors: India | China | Russia

Search.. Go

Hot Topics » IAEA-CIELO • TENDL-2019 • JENDL-5 • ENDF/B-VIII.0 News » Pointwise2020//TENDL-2019

## WIMS Library Update

Processing Documents Benchmarks Downloads Contributors

**NEWS!**

**28 November 2014**

- New **WIMSD libraries** were added based on the ENDF/B-VII.1 library.
- Some **programs, procedures and data files** were updated.
- **Plots** were updated.
- **New library documentation** was released.
- Temperature range extended up to 2000 K for actinides and fuel materials.
- Burn-up chains extended to higher actinides up to Cf-254.
- Bi-209 included as additional structural material.
- Dosimetry materials updated from IRDFF-v.1.05 or ENDF/B-VII.1 evaluated data.

**28 January 2008.**

- Due to a bug in NJOY processing multigroup data the WIMS-D library based on ENDF/B-VII data was incorrect. Only the Th-232 and Pa-231,233 data are affected.
- Corrected **WIMSD libraries** based on the ENDF/B-VII.0 data were uploaded.
- **Plots** were updated.
- The differences between the original and the corrected results for the standard benchmarks can be seen in [E70\\_bug.lst](#)

**Quick Links**

- ADS-Lib
- Atomic Mass Data Centre
- Beta-delayed neutrons
- CINDA
- Charged particle reference cross section
- CoNDERC
- DICEBOX
- DROSG-2000
- DXS
- Decay Data Library for Actinides
- EMPIRE-3.2
- ENDF Archive
- ENDF Retrieval
- ENDF-6 Codes
- ENDF-6 Format
- ENDVER
- ENSDF
- ENSDF ASCII Files
- ENSDF programs
- EPICS Electron & photon interaction data

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



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Search.. Go

Databases » ENSDF | XUNDL | NuDat | LiveChart | NSR | Nuclear Wallet Cards    Related » ENSDF Manuals | Codes | Nuclear Data Sheets | EXFOR

## Technical Meeting on Nuclear Data Processing

18-22 October 2021, IAEA Headquarters, Vienna, Austria

**Participants**

- Alexander Listov
- Beck Bret
- David Browne
- Oliver Buss
- Dermott E. Cullen
- Daniel Lopez Aldama
- Daniela Folgno
- Nathan Gibson
- Wim Haeck
- Andrew Holcomb
- Jaakko Leppanen
- Clement Jeannesson
- Cedric Jouanne
- Albert Kahler
- Do Heon Kim
- Luliz Leal
- Dieter Leichtle
- Mark Cornock
- Caleb M. Matoon
- Michael L. Zerkle
- Michael Fleming
- Morgan Lee
- Nicolas Leclaire
- Oscar Cabellos
- Paul Romano
- Marco T. Pigni
- Raphaelle Ichou

**Agenda**  
 The agenda is available [here](#).

**Summary Report**  
 The summary report is available as INDC(NDS)-0834.

**Background**  
 The Meeting is a follow-up of meeting of this subject in number of codes that can process evaluated nuclear data files.

**Objectives**  
 The overall objective of the IAEA Project is to validate continuous-energy Monte Carlo calculations. Specific objectives and best practices in data processing.

At the previous Meeting the results of the first phase of adequately process the cross sections and differential data. The generated ACE files were tested on a selected group, the calculated multiplication factors agreed to within the probability tables (or multi-band parameters) in the unit to 100 pcm due to different methods applied in different



International Atomic Energy Agency  
**Nuclear Data Services**  
 Provided by the Nuclear Data Section

IAEA.org | NDS Mission | Mirrors: India | China | Russia

Search.. Go

Databases » ENSDF | XUNDL | NuDat | LiveChart | NSR | Nuclear Wallet Cards    Related » ENSDF Manuals | Codes | Nuclear Data Sheets | EXFOR

## Technical Meeting on Nuclear Data Processing

23-26 September 2019, IAEA Headquarters, Vienna, Austria

**Participants**

- Bret Beck
- David Brown
- Cedric Jouanne
- Daniel Lopez Aldama
- Jeremy Conlin
- Kenichi Tada
- Ms Liu Ping
- Ms Raphaelle Ichou
- Oscar Cabellos
- Albert Kahler
- Tiejun Zu
- Alexander Listov
- Valentin Sinitza
- Ville Valtavirta
- Wim Haeck
- Wu Xiaofei
- Xu Jialong

**Scientific Secretary**  
 A. Trkov

**Contacts**

- R. Capote
- A. Koning
- J.-Ch. Sublet
- S. Okumura

**Agenda**  
 The Agenda is available [here](#).

**Background**  
 The Meeting is a follow-up of meeting of this subject in September 2018 ("TM on DP") and a previous meetings on this subject. A number of codes became available that can process evaluated nuclear data files. The focus is on (but not limited to) the ability to prepare data in ACE format for Monte Carlo calculations.

**Objectives**  
 The purpose of the Technical Meeting is to assess the current status and availability of nuclear data processing systems, with emphasis on their capability/capacity to support Monte Carlo calculations, including the treatment of self-shielding in the unresolved resonance region.

**Scope**

- The GNDS format as an alternative to the traditional ENDF format was essentially finalised. Information of the current status and development plans for codes that can process this format is needed.
- The code-verification project is in progress to validate codes that can generate libraries in ACE format. Results on the first stage (without self-shielding) were discussed at the previous meeting. Results on the second stage that includes self-shielding in the unresolved resonance range will be reported.
- Road-map for the next stage of testing the self-shielding treatment in the codes generating ACE files is to be laid out.
- Information on the status of other nuclear data processing codes is required.

**Presentations**

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

## □ Processing into JANIS format : HENDF – Hybrid ENDF files

- PENDF+MF2 (resonances)
- BOXER
- INTER

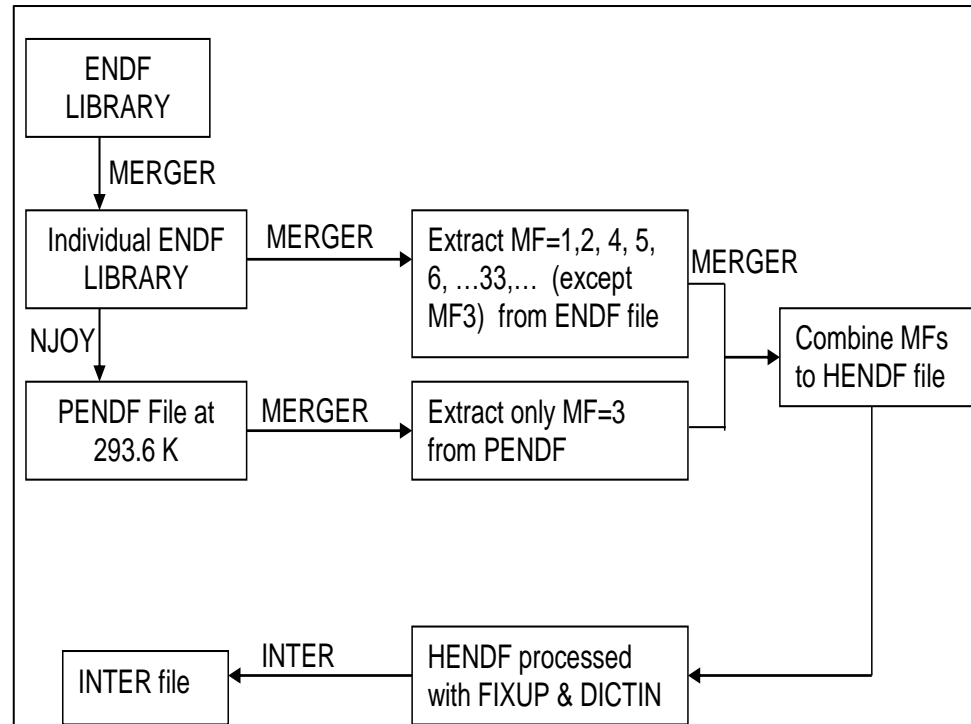
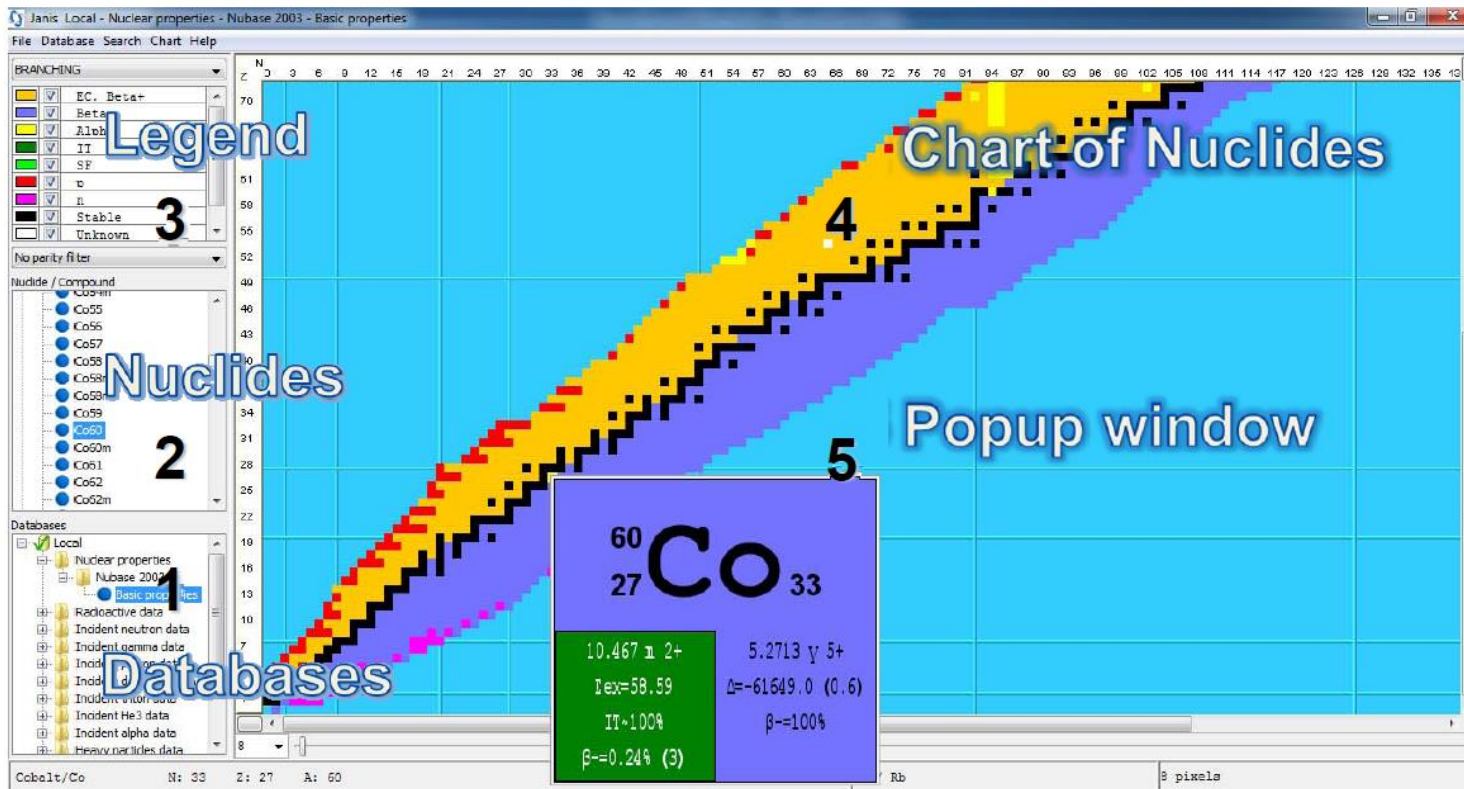


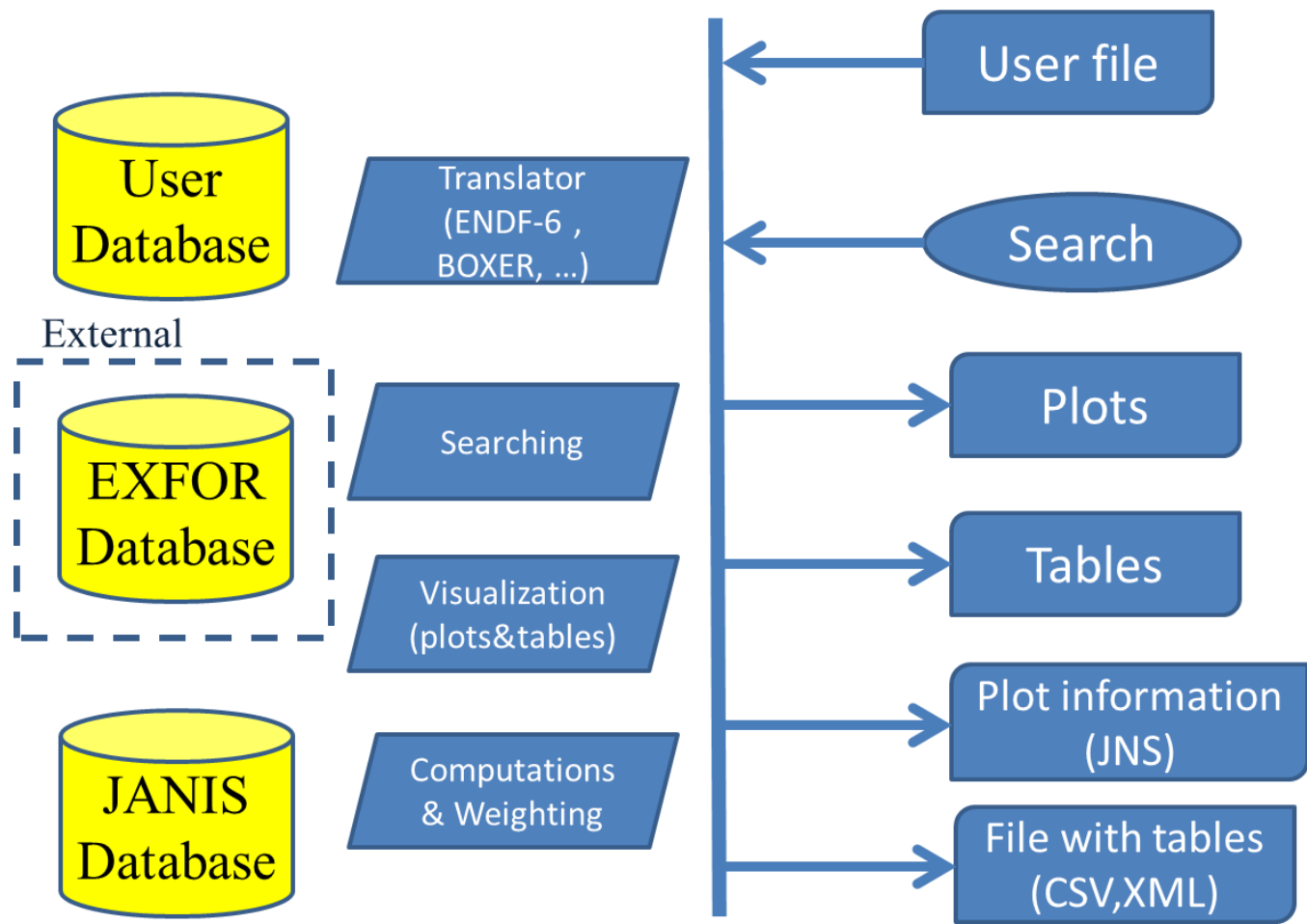
Figure. Flowchart of processing JANIS database from ENDF tapes

**J**ava-based **N**uclear Data Information **S**oftware designed to facilitate the visualisation and manipulation of nuclear data

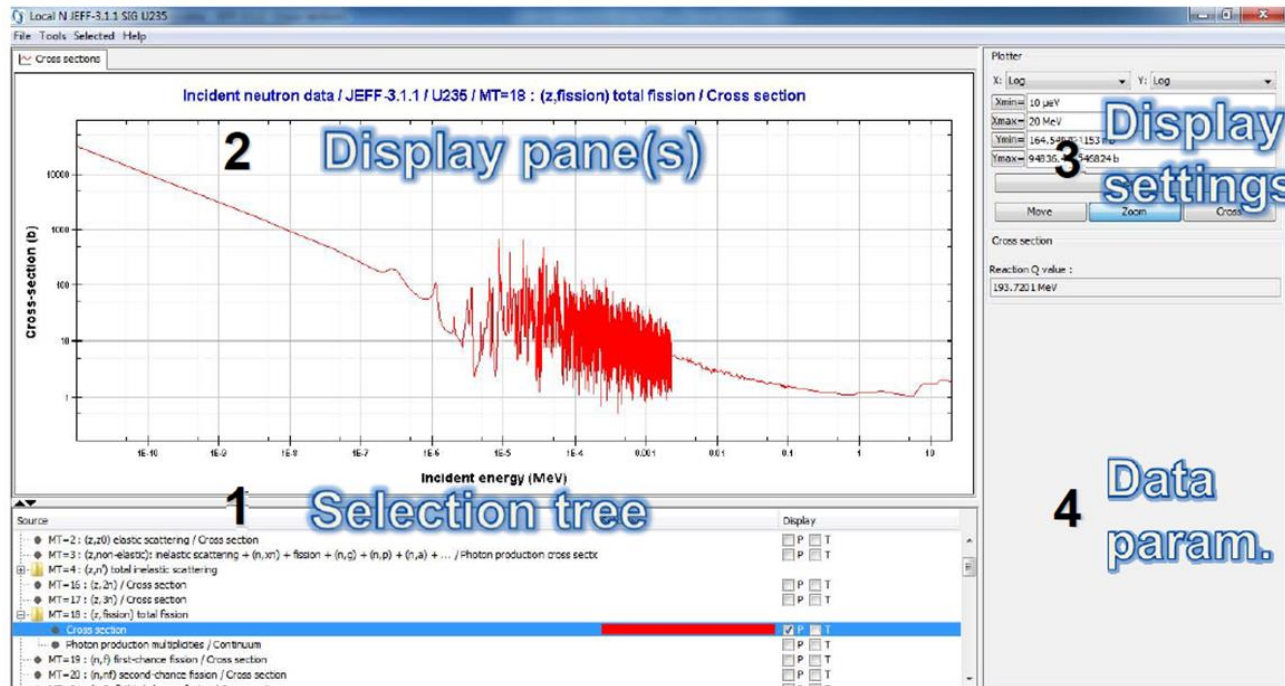


<http://www.oecd-nea.org/janis/>

- ❑ 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



## ➤ JANIS – Plot (renderer) window



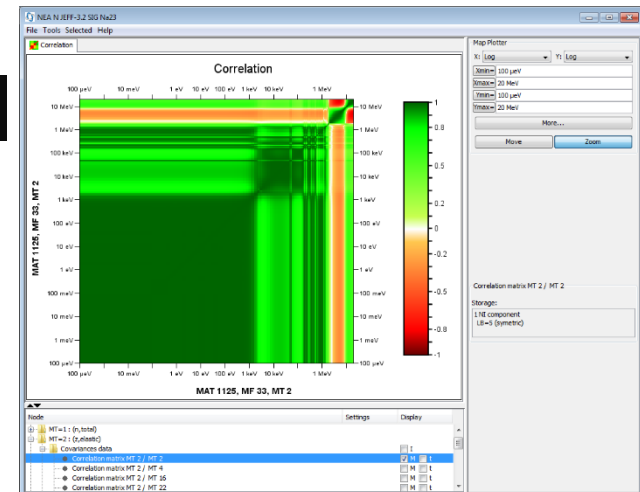
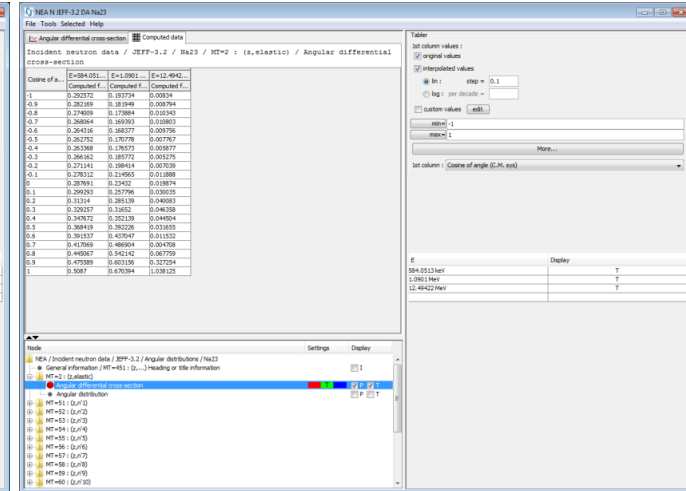
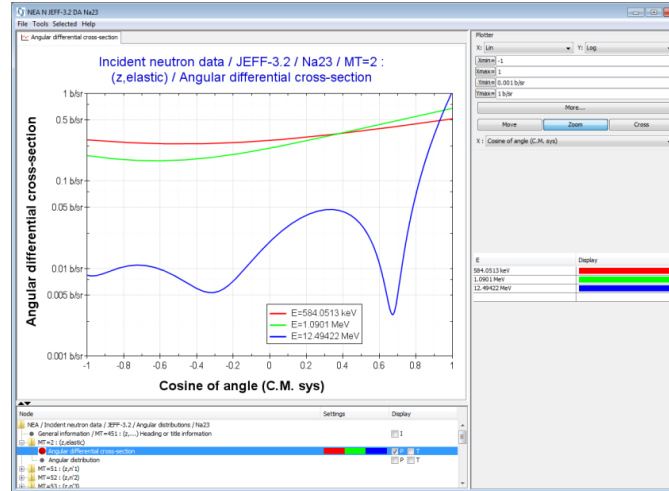
**1- Selection tree:** To select the data you want to display

**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..

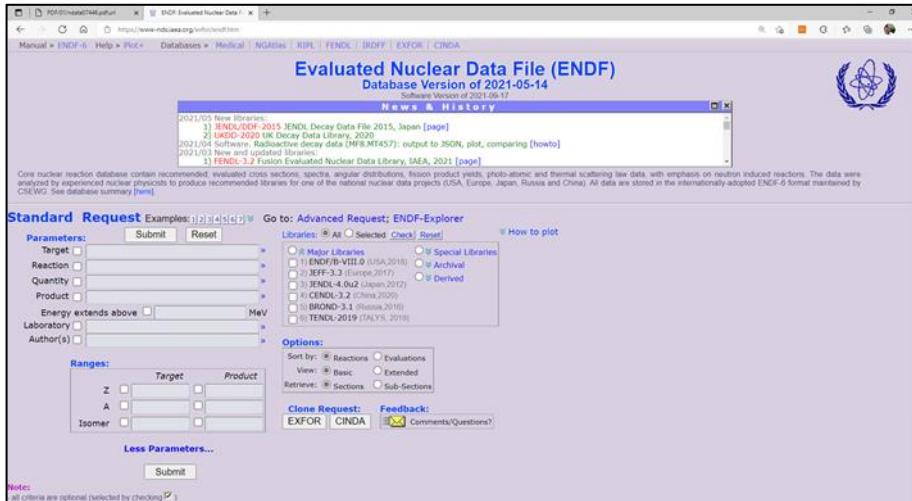
- **Others panels**
  - Text panels
  - Decay paths
  - Color maps
- **Save/Export**
  - JNS File to open
  - Figures in PNG or PS
- **Run command line**



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

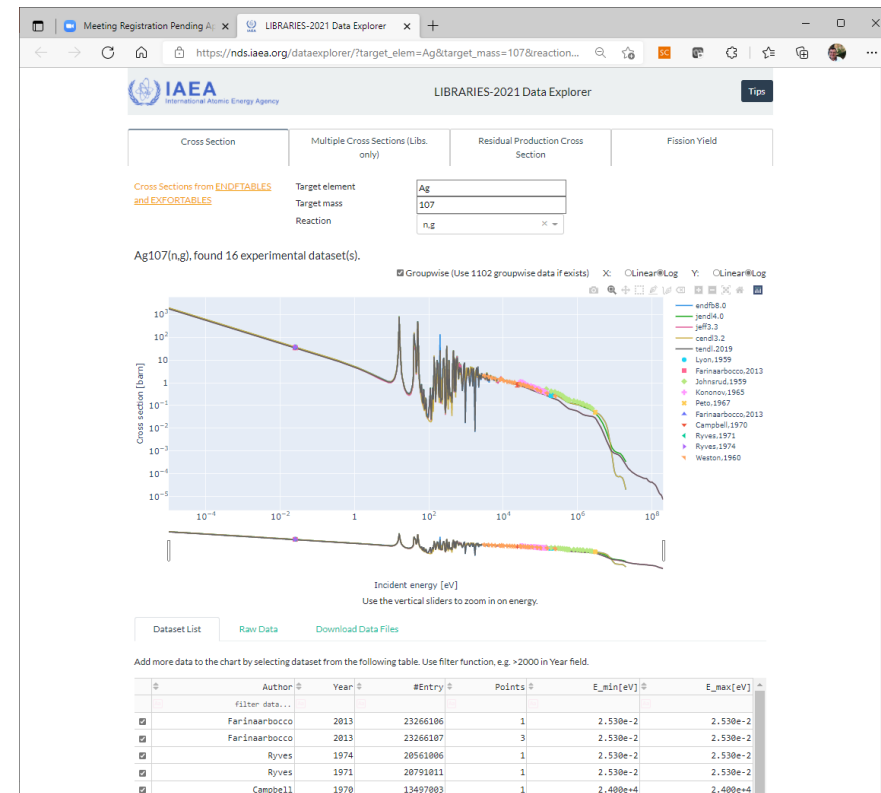


Figure. The IAEA/NDS retrieval system's website



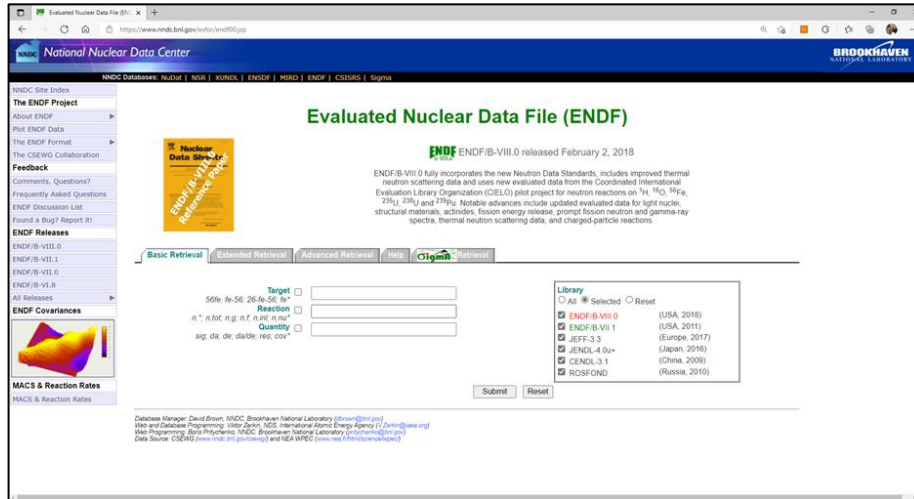
The screenshot shows the IAEA/NDS website interface for the Evaluated Nuclear Data File (ENDF) Database. The main heading is 'Evaluated Nuclear Data File (ENDF) Database Version of 2021-05-14'. Below this, there is a 'Standard Request' section with a 'Submit' button and a 'Reset' button. The 'Parameters' section includes fields for Target, Reaction, Quantity, Product, Energy extends above (MeV), Laboratory, and Author(s). There are also 'Ranges' for Z, A, and Isomer, and 'Options' for Sort by (Reactions, Evaluations), View (Basic, Extended), and Retrieve (Sections, Sub-Sections). A 'Clone Request' section includes 'EXFOR' and 'CINDA' buttons. A 'Feedback' section includes a 'Comments/Questions?' button.

<https://www-nds.iaea.org/exfor/endl.htm>



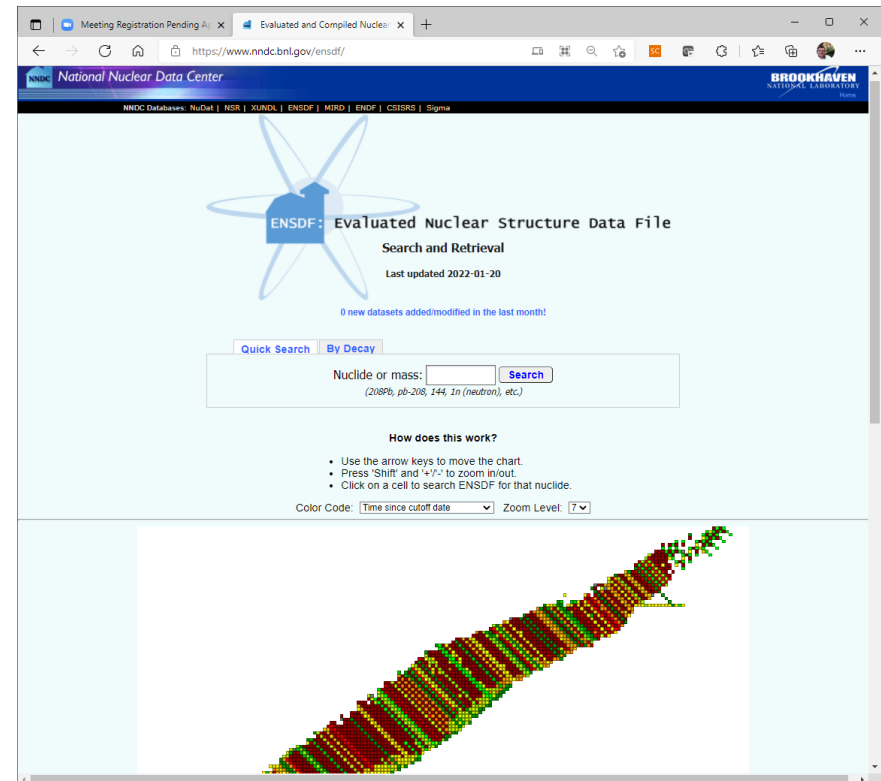
<https://nds.iaea.org/dataexplorer>

Figure. The NNDC retrieval system's website



<https://www.nndc.bnl.gov/exfor/endl00.jsp>

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



- ❑ *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*