

# Generation of SCALE Multi-Group Libraries with AMPX

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U.S. DEPARTMENT OF  
**ENERGY**

# ORNL nuclear data capabilities tightly coupled with M&S and nuclear applications

## **Analysis**

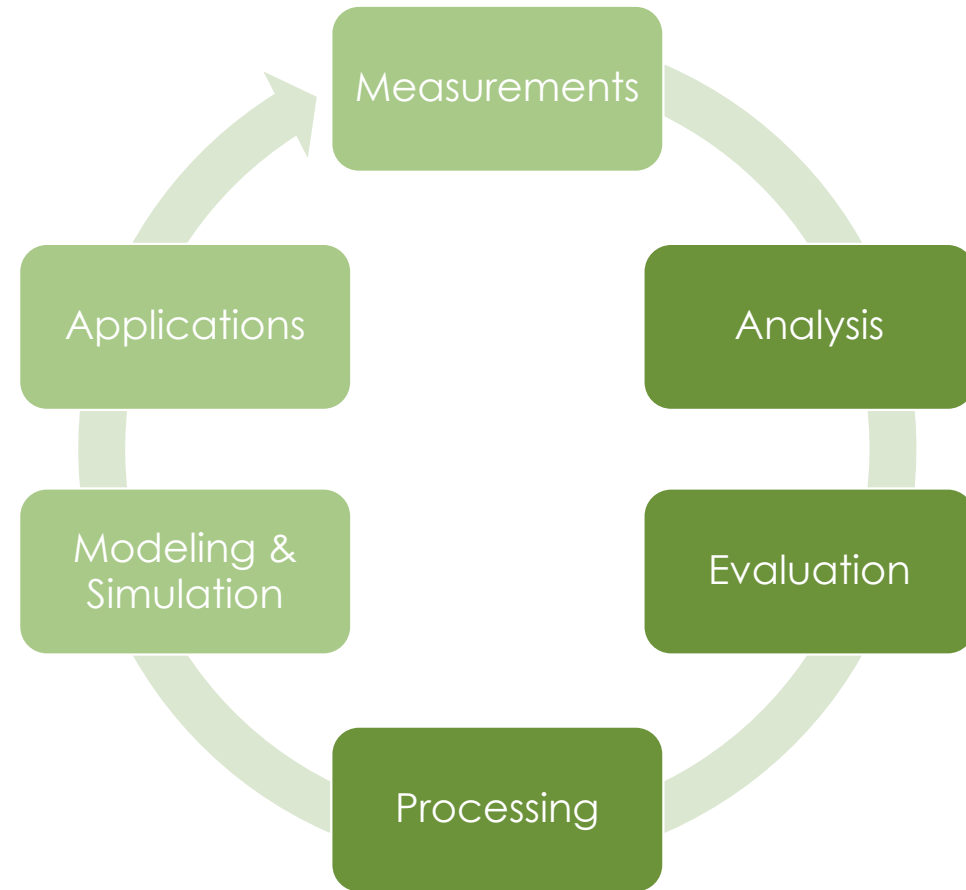
Nuclear data analysis methods development (SAMMY)

## **Evaluation**

Cross section evaluation and preparation of ENDF/B nuclear data files (SAMMY)

## **Processing**

Cross section processing methods development for generating nuclear data libraries (AMPX)



# AMPX Nuclear Data Processing History

- AMPX processes data in Evaluated Nuclear Data Files (ENDF) to provide CE, MG, Covariance, and ORIGEN Data Libraries for SCALE
- AMPX developed and maintained at ORNL for over 40 years
- 1990: ENDF Formats changed significantly with ENDF/B-VI release in 1990—AMPX could no longer process latest ENDF files for SCALE
- 1995—2002: Extensive AMPX upgrade to update AMPX to process latest ENDF/B data
- 2008-2012: AMPX upgrades for generation of continuous-energy shielding libraries
- 2002—2012: AMPX routinely processes latest ENDF/B Formats (e.g., ENDF/B-VI & –VII.0 data libraries in SCALE)
- 2012 – Present: Modernization effort to implement SQA and modern software design/development practices
- Current version available with SCALE 6.2 and up

Version	Year
ENDF/B-I	1968
ENDF/B-II	1970
ENDF/B-III	1972
ENDF/B-IV	1974
ENDF/B-V	1978
ENDF/B-VI	1990
ENDF/B-VII	2006
ENDF/B-VII.1	2011
ENDF/B-VIII.0	2018

# How to get data files

- ENDF - <http://www.nndc.bnl.gov/endl/b8.0/index.html>

The screenshot shows the NNDC website with a blue header. The main content area features the ENDF/B-VIII.0 logo and a headline: "Cross Section Evaluation Working Group (CSEWG) announces the release of the ENDF/B-VIII.0 evaluated nuclear reaction data library". Below this, a paragraph states: "On February 2, 2018, CSEWG released its latest revision of the ENDF/B library, ENDF/B-VIII.0." Another paragraph describes the updates: "ENDF/B-VIII.0 fully incorporates the new Neutron Data Standards, includes improved thermal neutron scattering data and uses new evaluated data from the Coordinated International Evaluation Library Organization (CIELO) pilot project for neutron reactions on  $^1\text{H}$ ,  $^{16}\text{O}$ ,  $^{56}\text{Fe}$ ,  $^{235}\text{U}$ ,  $^{238}\text{U}$  and  $^{239}\text{Pu}$ . The evaluations benefit from recent experimental data obtained in the U.S. and Europe, and improvements in theory and simulation. Notable advances include updated evaluated data for light nuclei, structural materials, actinides, fission energy release, prompt fission neutron and gamma-ray spectra, thermal neutron scattering data, and charged-particle reactions." A "Library summary" section follows, mentioning comparisons with ENDF/B-VII.0 and ENDF/B-VI.8. On the right, there is a section for "ENDF Reports and Documentation" featuring a yellow cover of the "Nuclear Data Sheets" with the text "ENDF/B-VIII.0 Reference Paper" overlaid. Below the cover are links to "ENDF/B-VIII.0 Issue of Nuclear Data Sheets" and "ENDF-6 Formats Manual (ENDF-102)". A left sidebar contains navigation links like "Search the NNDC:", "NNDC Site Index", "The ENDF Project", "About ENDF", "Plot ENDF Data", "The ENDF Format", "The CSEWG Collaboration", "ENDF/B-VIII.0", "ENDF/B-VIII.0 Home", "Special topics", "Download Library", "Other formats", "Errata", "How to Reference?", "ENDF-6 Format Specification", "Feedback", "Comments, Questions?", "Frequently Asked Questions", "ENDF Discussion List", "Found a Bug? Report it!", "ENDF/B Releases", "Related Projects", and "Beyond ENDF-6: GNDS". At the bottom, a table header is visible with columns: "No.", "NSUB", "Sublibrary", "Short", "VIII.0", "VII.1", "VII.0", "VI.8".

- JEFF - <https://www.oecd-neo.org/dbdata/jeff/>
- JENDL - <https://www.ndc.jaea.go.jp/jendl/j40/j40.html>
- Other data projects

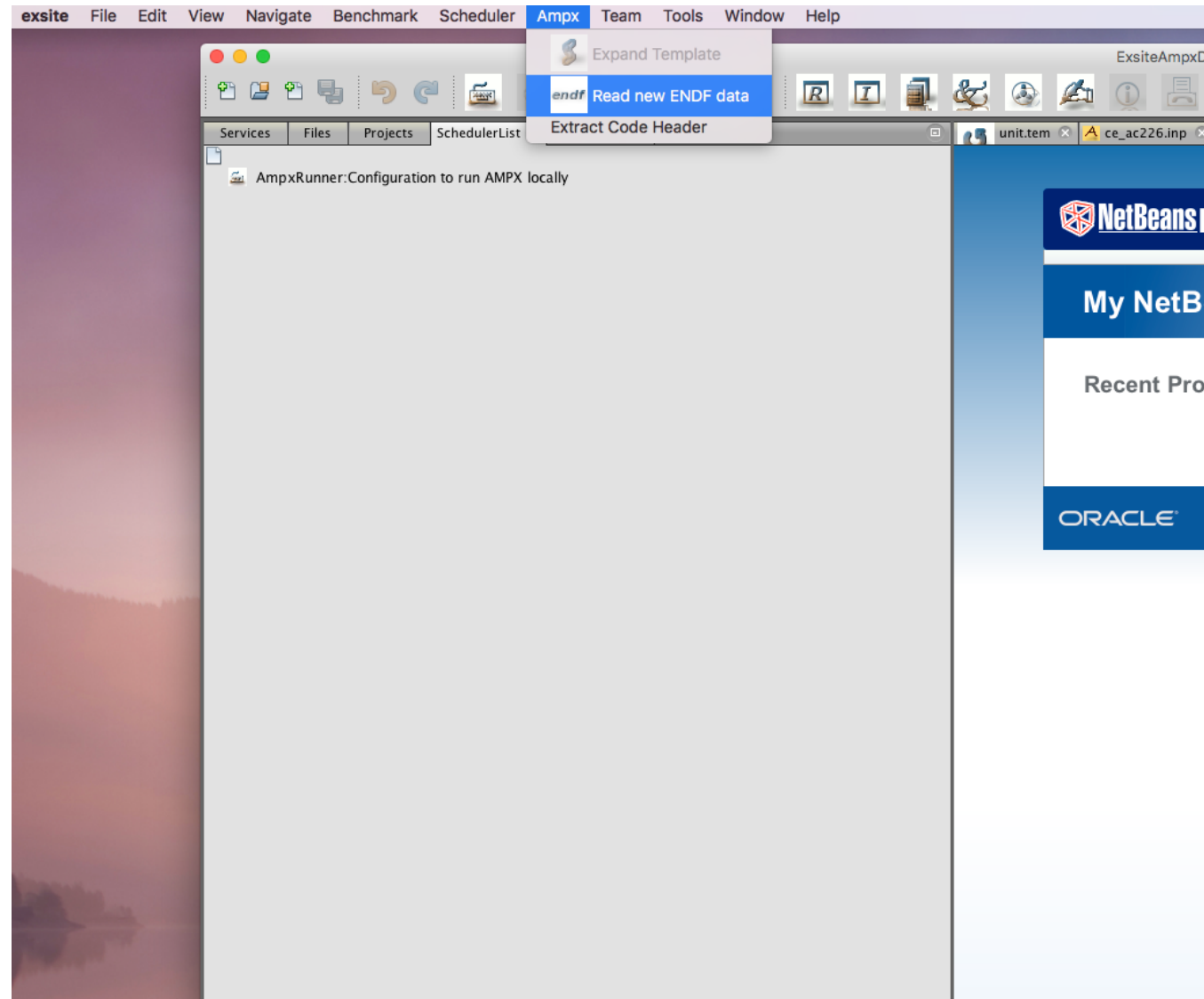
# ENDF sub libraries

NSUB	Sub library name	Short name	Use in AMPX
0	Photonuclear	g	
3	Photo-atomic	photo	Coupled MG/CE libraries
4	Radioactive decay	decay	Origen library data
5	Spont. fis. yields	sfy	Origen library data
6	Atomic relaxation	atom_relax	
<b>10</b>	<b>Neutron</b>	<b>n</b>	<b>MG/CE libraries</b>
11	Neutron fis. yields	nfy	Origen library data
<b>12</b>	<b>Thermal scattering</b>	<b>tsl</b>	<b>MG/CE libraries</b>
19	Standards	std	
113	Electro-atomic	e	
10010	Proton	p	
10020	Deuteron	d	
10030	Triton	t	
20030	<sup>3</sup> He	he3	
20040	<sup>4</sup> He	he4	

# Thermal scattering data

- Thermal scattering data exist in thermal range ( $<10\text{eV}$ ) only
- In fast range data for the corresponding stationary nuclide are used:
  - H1 in water: TSL data exist up to 5 eV (10eV in ENDF/B-VIII.0)
  - Above that use H1 data from neutron library
- In SCALE, we make two nuclides:
  - 8001001: H1 data from neutron library and free gas data in thermal range
  - 1001: H1 from TSL data in thermal range, H1 data from neutron library in fast range
- The connection between the fast and thermal data for thermal moderators needs to be done manually.
- Reliable automatic detection is not possible as the ENDF files do not provide enough information.

# Open ExSite Generate XML listing.





# XML ENDF listing

```
<Material AWP0="yes"
  author="IAEA CIELO Collaboration"
  awi="1.0"
  awr="233.0248"
  chicov="yes"
  covariances="yes"
  dbrcnuclide="yes"
  dist="DIST-FEB18"
  ehRes="2.25000E+03"
  endf="9228"
  eval="EVAL-NOV17"
  file12="yes"
  file2="yes"
  file3="yes"
  file4="yes"
  file5="yes"
  file6="yes"
  file8="yes"
  file9_10="yes"
  filename="n-092_U_235.endf"
  fission="yes"
  gamma="no"
  lab="IAEA"
  lis="0"
  liso="0"
  metaStable="false"
  mod="1"
  neutron="yes"
  nis="1"
  nlib="0"
  pureAbsorber="no"
  rdate=""
  rel="0"
  resolved="yes"
  resonance="RM"
  rev="8"
  scattering="1.15860E+01"
  tag="u235"
  tape="/endf7/neutrons/n-092_U_235.endf"
  totalFission="yes"
  unresolved="yes"
  version="6"
  za="92235"
  zai="1"
/>
```



# Examine \_config file

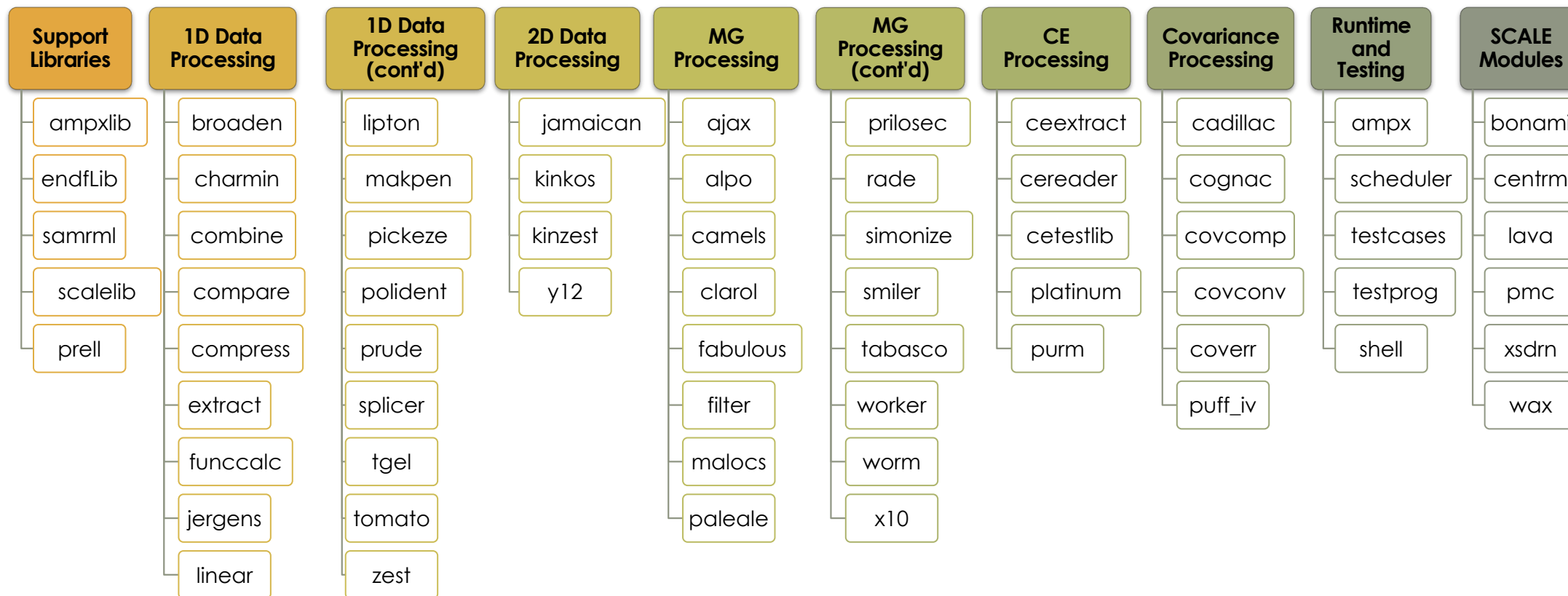
```
<metastable>
  <nuclei endf="1323" realza="13026" scaleza="1013026" /> <!-- Metatable al26m1 uses SCALE ID=1013026 -->
  <nuclei endf="9547" realza="95242" scaleza="1095242" /> <!-- Metatable am242m1 uses SCALE ID=1095242 -->
</metastable>

<!-- nuclei for which the scale id is different from the real za value -->
<specialNuclei>
  <nuclei endf="125" realza="1001" scaleza="8001001" name="hfreegas" /> <!-- for h1 SCALE uses ID=8001001 -->
  <nuclei endf="128" realza="1002" scaleza="8001002" name="dfreegas" /> <!-- for h2 SCALE uses ID=8001002 -->
</specialNuclei>

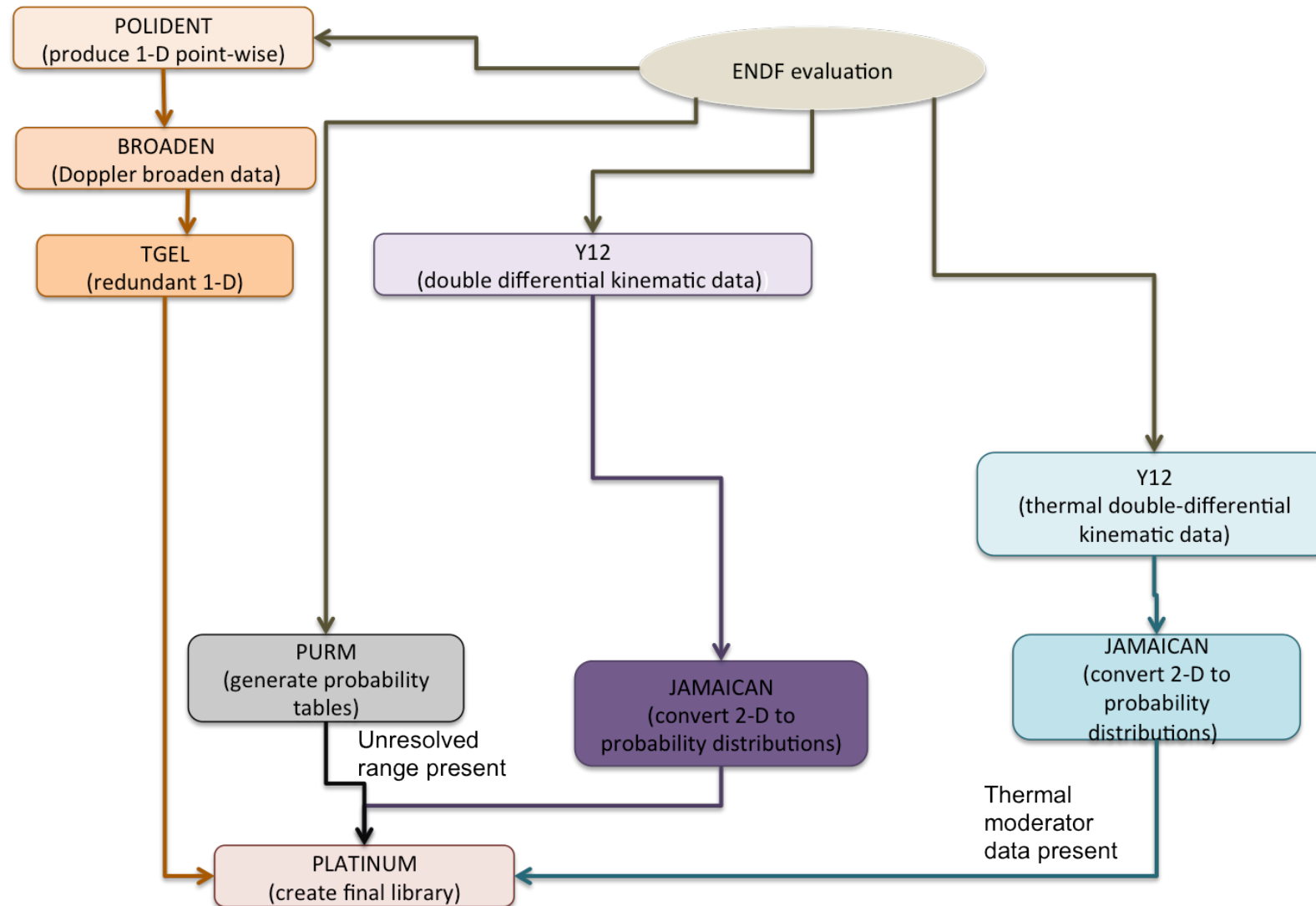
<!-- thermal nuclei -->
<thermal>
  <nuclei endf="1" realza="1001" > <!-- thermal evaluation h_h2o -->
    <fastMat endf="125" scaleza="1001" name="h-1" /> <!-- bound with fast evaluation h1 uses SCALE ID=1001 -->
  </nuclei>

  <nuclei endf="30" realza="130" > <!-- thermal evaluation graphite -->
    <fastMat endf="625" scaleza="3006012" name="graphite" /> <!-- uses SCALE ID=6312 -->
    <fastMat endf="628" scaleza="3006013" name="graphite" /> <!-- uses SCALE ID=6312 -->
  </nuclei>
</thermal>
```

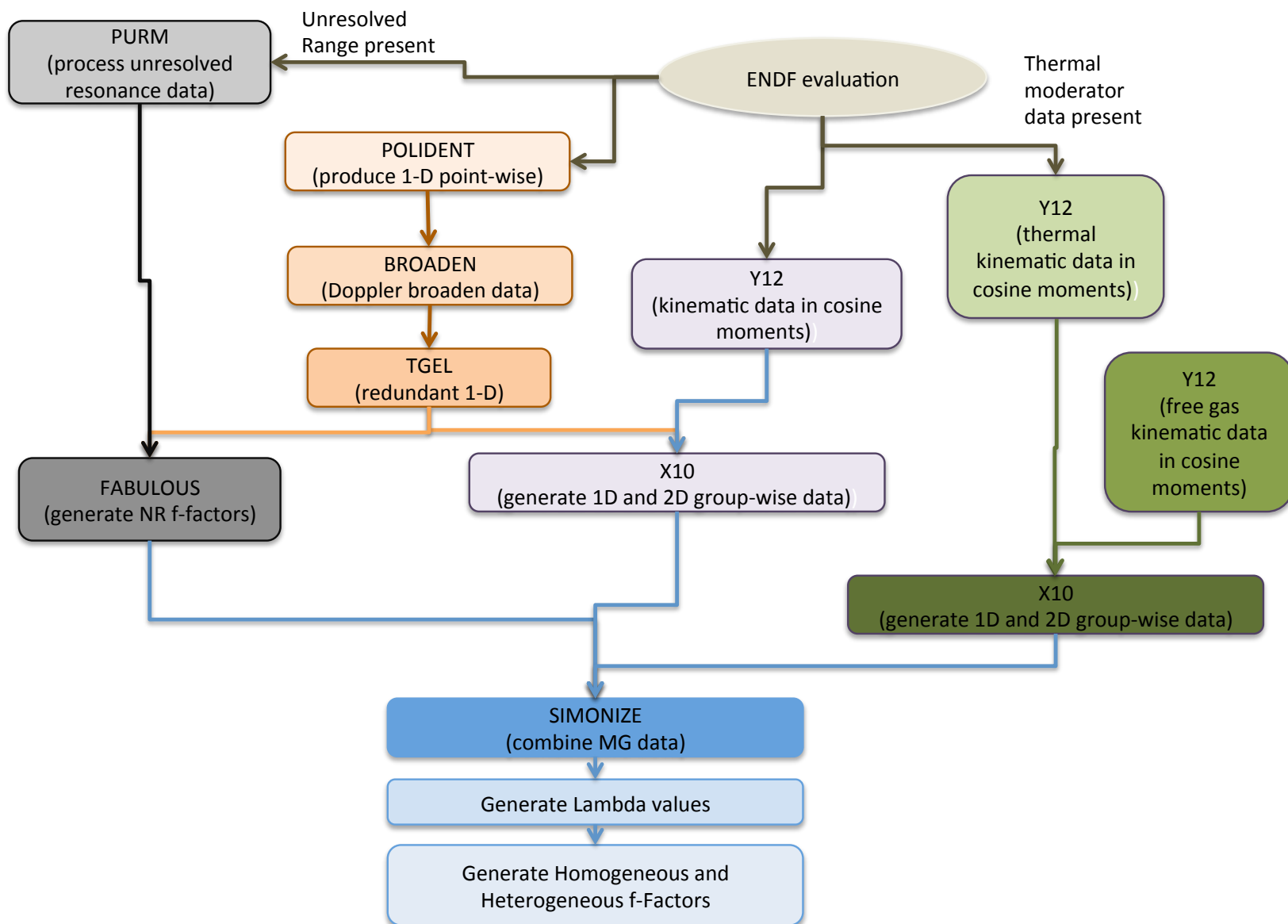
# AMPX Modular Code System



# Processing CE Libraries



# Processing MG Libraries



# Point1d expansion

Configure point1d

Use: ☒ **point**    
Output file name for point data. A unique tag name for the nuclide will be appended.

Use: ☐ **eps**   
Precision to which to create the grid in the resolved resonance range.

Use: ☒ **broaden**    
Output file name for broadened data. A unique tag name for the nuclide will be appended.

Use: ☒ **temperatures**   
List of temperatures to broaden the data to (K).

Use: ☐ **reactions**   
List of MTs to broaden. By default 1 (total), 2 (elastic), 18,19,20,21 and 38 (fission) and 102 (capture) are broadened

Use: ☐ **mt\_option**    
Add additional reaction values to be broadened

Use: ☒ **input**    
Name of the AMPX input files to create. Tag name will be appended

Use: ☒ **evals**    
Pick Endf xml summary listing or an endf file

Use: ☒ **absolute** ☒  
Should files names in the input file appear as typed

# P-table expansion

Configure ptable

Use: ☒ ptableloc

Name for the probability table files.

Use: ☒ temps

The temperature at which to create the probability tables.

Use: ☐ sig0

The sig0 values at which to calculate Bondarenko factors.

Use: ☐ dofile7

Make continuous energy data for moderator materials (ENDF evaluation contains File 7)

Use: ☒ input

Name of the AMPX input files to create. Tag name will be appended

Use: ☒ evals

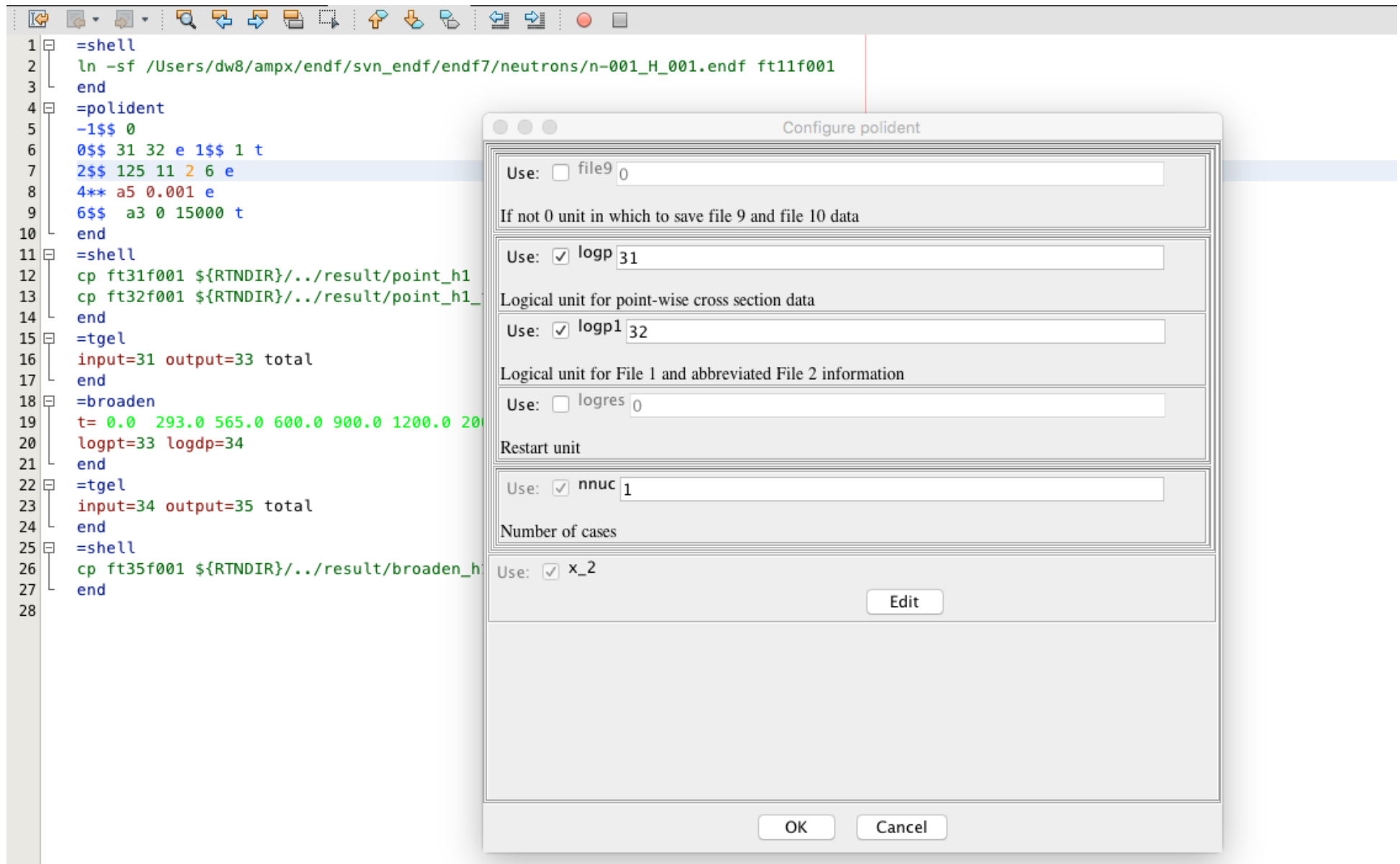
Pick Endf xml summary listing or an endf file

Use: ☒ absolute ☒

Should files names in the input file appear as typed

OK Cancel

# Examine the input files



The image shows a code editor window with a list of input files on the left and a 'Configure polident' dialog box on the right. The code editor displays a series of commands for setting up a simulation, including file creation, directory setup, and parameter assignment. The 'Configure polident' dialog box is used to configure the simulation parameters, with fields for file names, logical units, and restart units.

```
1 =shell
2 ln -sf /Users/dw8/ampx/endl/svn_endl/endl7/neutrons/n-001_H_001.endl ft11f001
3 end
4 =polident
5 -1$$ 0
6 0$$ 31 32 e 1$$ 1 t
7 2$$ 125 11 2 6 e
8 4** a5 0.001 e
9 6$$ a3 0 15000 t
10 end
11 =shell
12 cp ft31f001 ${RTNDIR}/../result/point_h1
13 cp ft32f001 ${RTNDIR}/../result/point_h1
14 end
15 =tgel
16 input=31 output=33 total
17 end
18 =broaden
19 t= 0.0 293.0 565.0 600.0 900.0 1200.0 20
20 logpt=33 logdp=34
21 end
22 =tgel
23 input=34 output=35 total
24 end
25 =shell
26 cp ft35f001 ${RTNDIR}/../result/broaden_h1
27 end
28
```

**Configure polident**

Use: ☐ file9 0

If not 0 unit in which to save file 9 and file 10 data

Use: ☒ logp 31

Logical unit for point-wise cross section data

Use: ☒ logp1 32

Logical unit for File 1 and abbreviated File 2 information

Use: ☐ logres 0

Restart unit

Use: ☒ nnuc 1

Number of cases

Use: ☒ x\_2

Edit

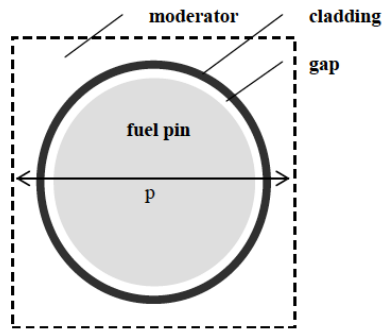
OK Cancel



# Flux selection

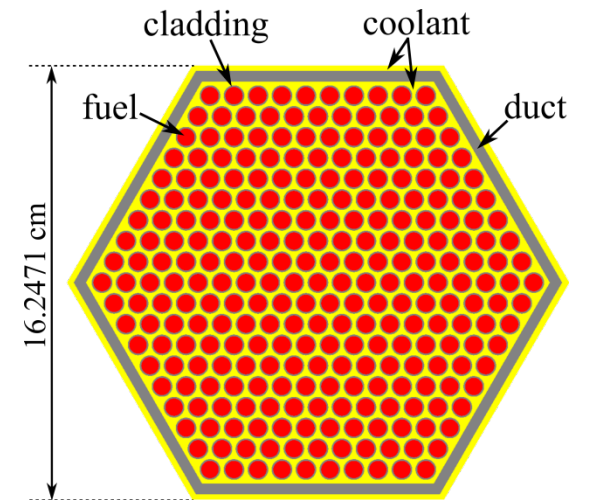
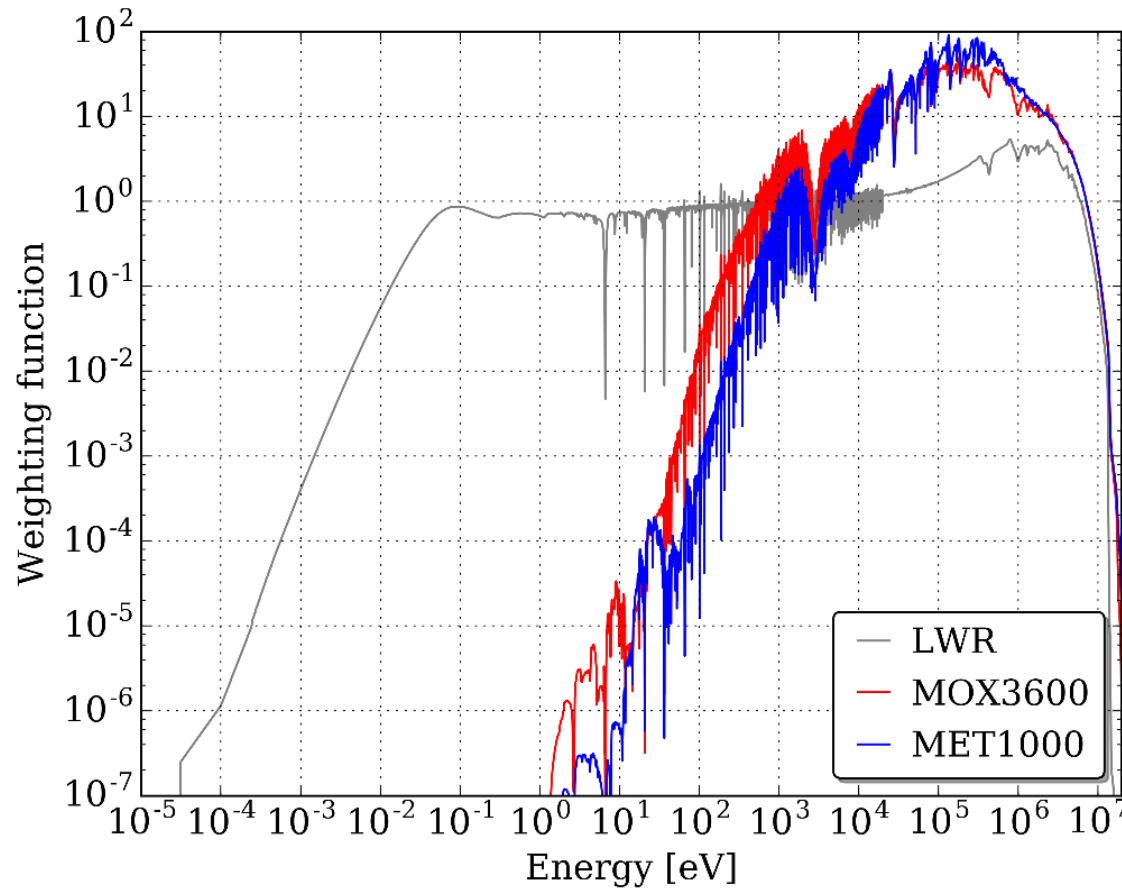
- Flux is just a 1-D function over Energy in eV.
- Any 1-D function can be used (there are programs that convert to ASCII (x,y) values to the needed binary file).
- Flux can be temperature and ZA dependent.
- Flux can be generated from a CENTRM run.
- For the tutorial we are using the standard weighting function

# Flux choices

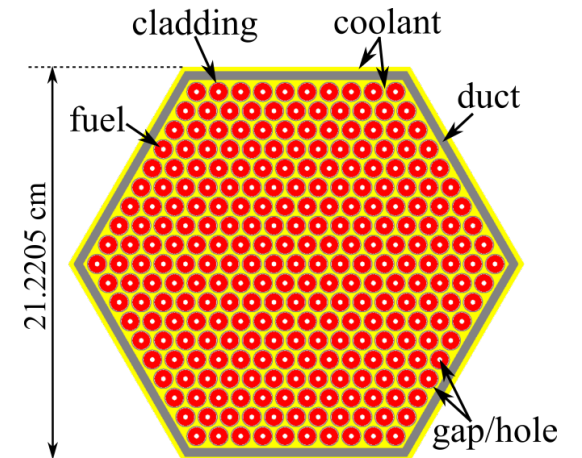


p – pitch of the unit cell

**LWR pin cell**



**MET1000 fuel assembly**



**MOX3600 fuel assembly**

# Homogenized SFR fuel assembly

MG library	$k_{\infty}$	$\Delta\rho = (1/k_{\text{ref}} - 1/k_{\infty})$ [pcm]
CE	1.27539(11)	(ref)
252g, LWR	1.27047(8)	-304(14)
230g, MET1000	1.27865(8)	200(14)
230g, MOX3600	1.27694(8)	95(14)
302g, MET1000	1.27659(8)	74(14)
302g, MOX3600	1.27563(8)	15(14)
2082g, MET1000	1.27560(8)	13(14)
2082g, MOX3600	1.27513(8)	-16(14)

## 252g LWR:

- group structure optimized for thermal systems
- weighting function LWR spectrum
- SCALE standard library

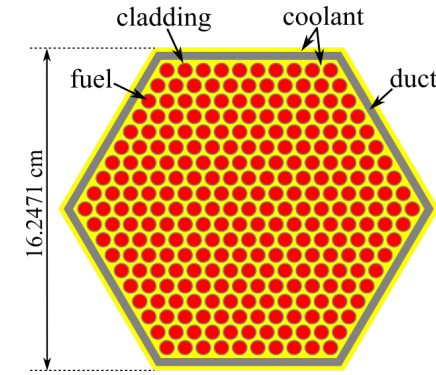
## Others:

- group structure optimized for SFR systems
- two different SFR weighting spectra

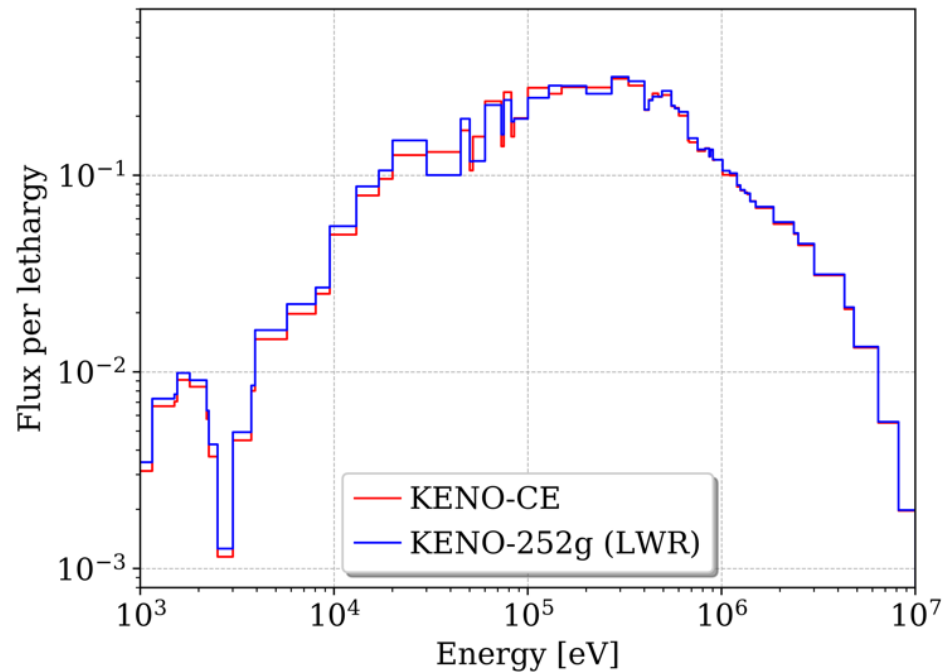
Influence of  
weighting spectrum

Influence of energy  
group structure

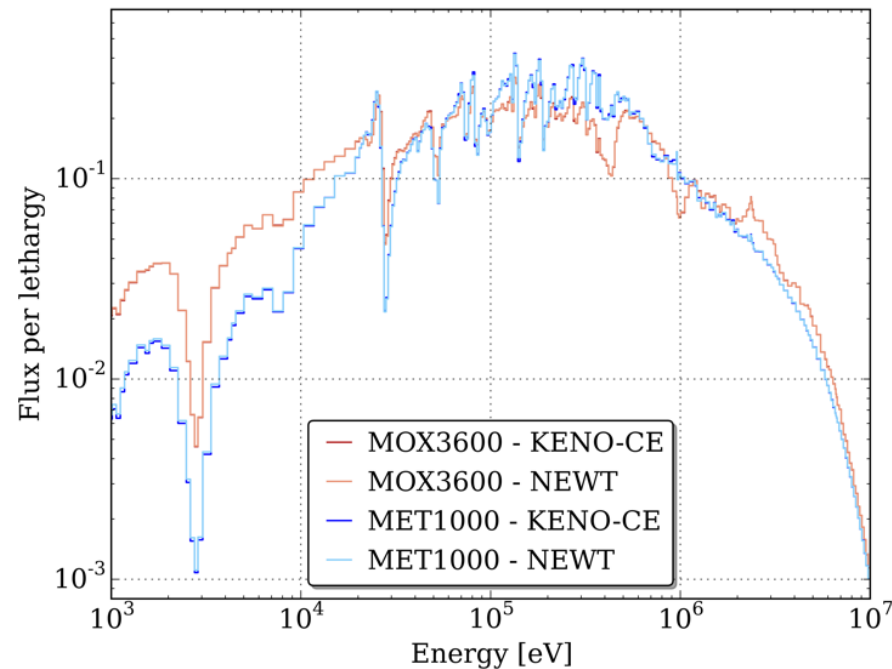
# Neutron flux of a homogenized SFR fuel assembly



**MET1000**



**KENO 252g calculation**



**KENO 302g (SFR) calculation**

# Some VALID calculations

Experiment	Measurement	CE	252g	302g	$\Delta k$ (252g vs. CE) [pcm]	$\Delta k$ (302g vs. CE) [pcm]
HEU-MET-FAST-021-001	1.0000(24)	0.9963(1)	1.0069(1)	1.0006(1)	1067	431
HEU-MET-FAST-040-001	0.9991(11)	1.0045(1)	1.0081(1)	1.0057(1)	362	117
PU-MET-FAST-026-001	1.0000(24)	0.9969(1)	1.0053(1)	1.0005(1)	834	360
IEU-MET-FAST-005-001	1.0000(21)	1.0012(1)	1.0124(1)	1.0054(1)	1127	423
IEU-MET-FAST-006-001	1.0000(23)	0.9961(1)	1.0016(1)	0.9972(1)	549	111
LEU-COMP-THERM-002-004	0.9997(20)	0.9986(1)	0.9986(1)	1.0652(1)	-2	6652
LEU-COMP-THERM-002-005	0.9997(20)	0.9974(1)	0.9972(1)	1.0713(1)	16	7402

**It is important to choose a group structure and weighting spectrum appropriate for the system under investigation!**

# MG template

Configure neutron\_mg

Use: ☒ master

**Invalid value: File name cannot be empty**  
File name for the AMPX master to generate. A unique tag name for the nuclide will be appended.

Use: ☒ temperature

**Invalid value: null**  
The temperature at which to create the master. The selected temperature has to exist in the broadened data files.

Use: ☒ broaden

**Invalid value: File name cannot be empty**  
File name for broadened data. The data are assumed to exist. A unique tag name for the nuclide will be appended. The file needs to contain point data broadened to the temperature given in temperature variable.

Use: ☒ neutgroups

**Invalid value: Unable to parse as a Integer**  
Number of neutron groups to use.

Use: ☒ thermalgroups

**Invalid value: Unable to parse as a Integer**  
Number of thermal groups.

Use: ☐ neutuserdef

Use: ☐ neutbounds

Energy boundaries for the neutron groups (eV)

Use: ☐ gamgroups

Number of gamma groups to use.

Use: ☐ gamuserdef

Use: ☐ gambounds

Energy boundaries for the gamma groups (eV)

Use: ☐ weightuser

Use: ☐ weighting

Weighting function to use to create multigroup data

Use: ☐ tmax

Temperature of Maxwellian spectrum in weighting function (K) if the weighting function contains a Maxwellian part. If a Watt fission spectrum is generated this is the value of a.

Use: ☐ akt

Cut-off energy in eV up to which Maxwellian is used:  $tmax * akt * 8.61664e-5$  if the weighting function contains a Maxwellian part. If a Watt fission spectrum is generated this is the value of b.

# Bondarenko Factors

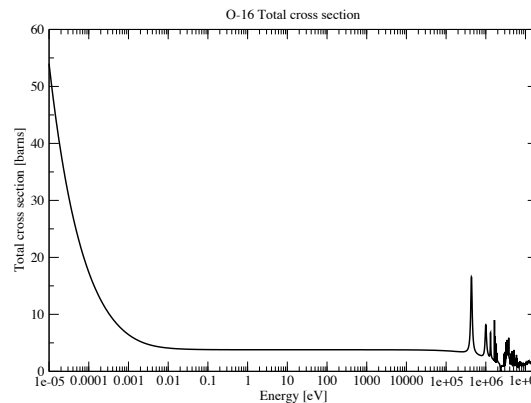
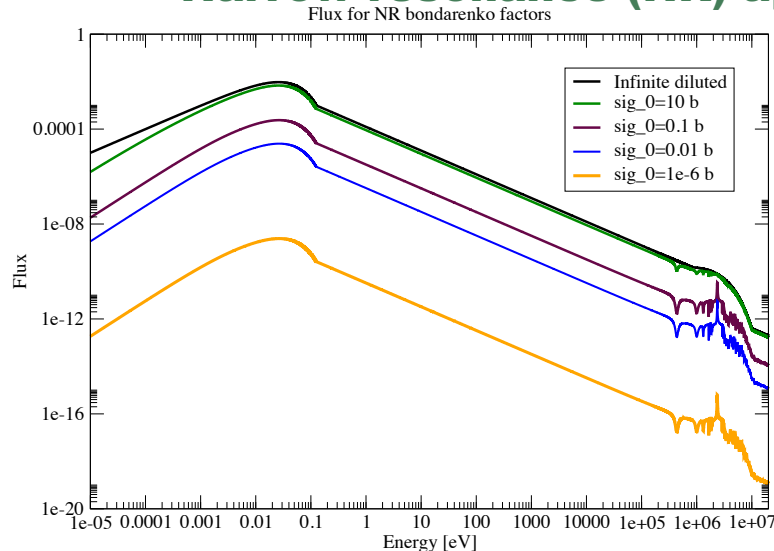
Calculate problem independent cross section data as a function of background cross section and temperature:

$$\sigma_{x,g}^{(j)}(\sigma_0, T) = \frac{\int_g \sigma_x^{(j)}(E, T) \varphi(E, \sigma_0, T) dE}{\int_g \varphi(E, \sigma_0, T) dE}$$

Divide by a reference cross section to get factors

In a shielding calculation, determine desired background cross section and interpolate the factor from tabulated factors

## Narrow resonance (NR) approximation



$$\varphi(E, \sigma_0, T) = \frac{\sigma_0 \varphi_{ref}(E)}{\sigma_t^{(j)}(E, T) + \sigma_0}$$

Flux for  $^{16}\text{O}$  for different background values



# Homogenous F-Factor for Intermediate Resonance Treatment

Our Multi-Group libraries contain homogenous f-factors for nuclides with  $A > 40$  in the resolved resonance range. These are intermediate resonance (IR) f-factors. Otherwise NR f-factors are used.

Use modules PMC and CENTRM to calculate a shielded cross section, with a CE flux for a homogenous model

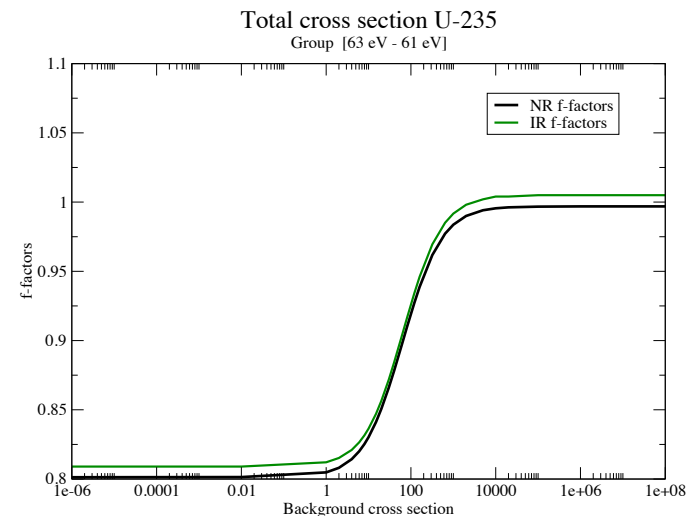
$$\left( \sigma_t^{(j)}(E, T) + \sigma_0 \right) \varphi(E, \sigma_0, T) = \int_E^{E/\alpha^{(j)}} \frac{\sigma_s^{(j)}(E', T) \varphi(E', \sigma_0, T)}{(1 - \alpha^{(j)}) E'} dE' + \sigma_0 \int_E^{\infty} \frac{\varphi(E', \sigma_0, T)}{E'} dE'$$

$1 - \alpha^{(j)}$  = the maximum fractional energy loss in an elastic collision with nuclide  $j$ ;

$\sigma_0 = \frac{N^{(H)}}{N^{(j)}} \sigma_p^{(H)}$  (the background cross section);

$\sigma_p^{(H)}$  = the potential cross section for hydrogen;

If the desired scattering nuclide is not fissionable, a small amount of u-235 is added to the homogenous model



# Bondarenko template

Configure bondarenko\_prob

Use: ☒ master    
**Invalid value: File name cannot be empty**  
File name for master containing full range bondarenko data. A unique tag name for the nuclide will be appended.

Use: ☒ broaden    
**Invalid value: File name cannot be empty**  
File name for broadened data. A unique tag name for the nuclide will be appended. These data are assumed to already be calculated and are used to determine the reference temperature.

Use: ☒ n1d    
**Invalid value: File name cannot be empty**  
File name for master containing 1D neutron data to be used as references data. It is assumed to exist. A unique tag name for the nuclide will be appended.

Use: ☒ prob    
**Invalid value: File name cannot be empty**  
File name for the probability tables

Use: ☒ temperature   
**Invalid value: null**  
The temperature at which the reference data are given

Use: ☐ weightuser    
Use a standard AMPX weighting function

Use: ☐ weighting    
Weighting function to use to create multigroup data

Use: ☐ tmax   
Temperature of Maxwellian spectrum in weighting function (K) if the weighting function contains a Maxwellian part. If a Watt fission spectrum is generated this is the value of a.

Use: ☐ akt   
Cut-off energy in eV up to which Maxwellian is used:  $tmax * akt * 8.61664e-5$  if the weighting function contains a Maxwellian part. If a Watt fission spectrum is generated this is the value of b.

Use: ☐ theta   
Effective temperature in eV of the fission spectrum Only used if weighting function contains a Maxwellian part)

Use: ☐ fcut   
Point at which to join 1/E to fission spectrum (eV). Only used if weighting function contains a Maxwellian part)

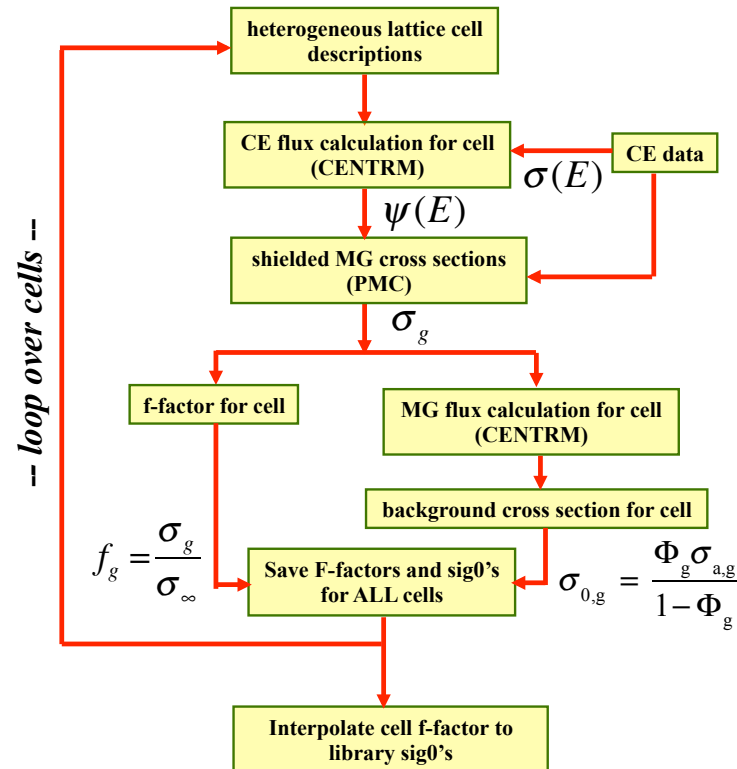
Use: ☐ el   
Lower limit in eV of the weighting spectrum.

Use: ☐ eh   
Upper limit in eV of the weighting spectrum.

# Heterogenous F-Factor for Intermediate Resonance Treatment

Similar to homogeneous f-factors, but:

- Heterogenous models are now used
- Background cross section can not be determined in advance
- A suite of predefined models is used



# Within Group Scattering F-Factors

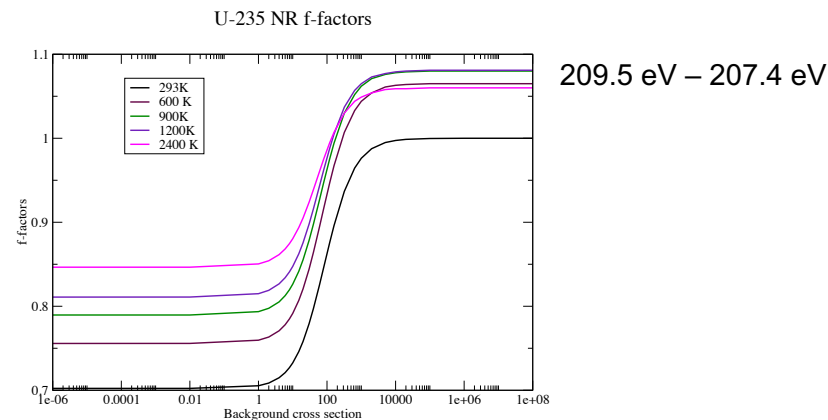
In order to account better for in-group elastic scattering, f-factors (NR and IR) can be added to a MG library.

For NR:

- Calculate the diagonal elements of the elastic scattering matrix, using the NR flux.
- Calculate f-factor using the diagonal element of the elastic scattering matrix as a reference factor

For IR:

- The same procedure is used as for other homogeneous or heterogeneous f-factors.
- PMC generates a model dependent scattering matrix.
- Calculate f-factors using the diagonal element of the shielded matrix and the the elastic scattering matrix as a reference factor.



# Bind the library for each nuclide

```
Start Page x test.tem x A bind_h_h2o_thermal.inp x
1 =shell
2   ln -sf ${RTNDIR}/../result/neut_neutron_h1 ft01f001
3   ln -sf ${RTNDIR}/../result/bond_h_h2o_h1 ft03f001
4   cp ft03f001 ft33f001
5   ln -fs ${RTNDIR}/../result/neut_h_h2o_thermal_1001 ft04f001
6   end
7 =filter
8   in=4 out=44 ldn mt=1007 1008
9   end
10 =simonize
11   Identifier=1001 master=20
12   title= h_h2o 1 fast: h1 endf-8 REL0 REV8 MOD0
13   za=10010
14   fastid=8000125 thermid=8000001 source=0 BONDARENKO=3 id19=125
15   ldn=33 id19=125
16   2dn=4 id19=1001 MT=0 MODERATOR
17   ldn=44 id19=1001
18
19   neutron=1 id19=125
20   end
21
22 =ajax
23   0$$ 21 e 1$$ 1 t
24   2$$ 20 0 e t
25   h_h2o 1 fast: h1 endf-8 REL0 REV8 MOD0
26   end
27 =rade
28   1$$ 21 e t
29   end
30 =shell
31   cp ft21f001 ${RTNDIR}/../result/master_h_h2o_h1
32   end
33
```

# Make an AMPX master library

Configure combine\_mgs

Use: ☒ master

Final master/working library

Use: ☒ indmaster

File containing neutron master or working library. Tag name of isotope is automatically appended

Use: ☐ dofile7

Include thermal moderator files

Use: ☐ iswork

Do you want to combine working libraries

Use: ☐ title1

First title line for the final master/working library

Use: ☐ title2

Second title line for the final master/working library

Use: ☒ input

Name of the AMPX input files to create. Tag name will be appended

Use: ☒ evals

Pick Endf xml summary listing or an endf file

Use: ☐ absolute ☐

Should files names in the input file appear as typed

# Verification

- We now have a library that can be used with SCALE, but we have not tested it.



# Simple SCALE input data to test each nuclide

Configure allnucinf

Use: ☒ master

Library name

Use: ☐ parm centrm

Parameter string for csas sequence

Use: ☐ celibrary Testing a multigroup library

Use: ☐ temp 300

Temperature at which to do the calculation

Use: ☐ dofile7 yes

Generate input files for thermal moderators

Use: ☐ spectrum thermal

Which flux to use

Use: ☐ usershell pwd

Any shell commands you may want to prefix the run with

Use: ☐ gen 1100

Number of total generations

Use: ☐ nsk 100

Number of skipped generations

Use: ☐ npg 5000

Number of particles per generation

Use: ☒ input

Name of the AMPX input files to create. Tag name will be appended

Use: ☒ evals

Pick Endf xml summary listing or an endf file

Use: ☐ absolute ☐

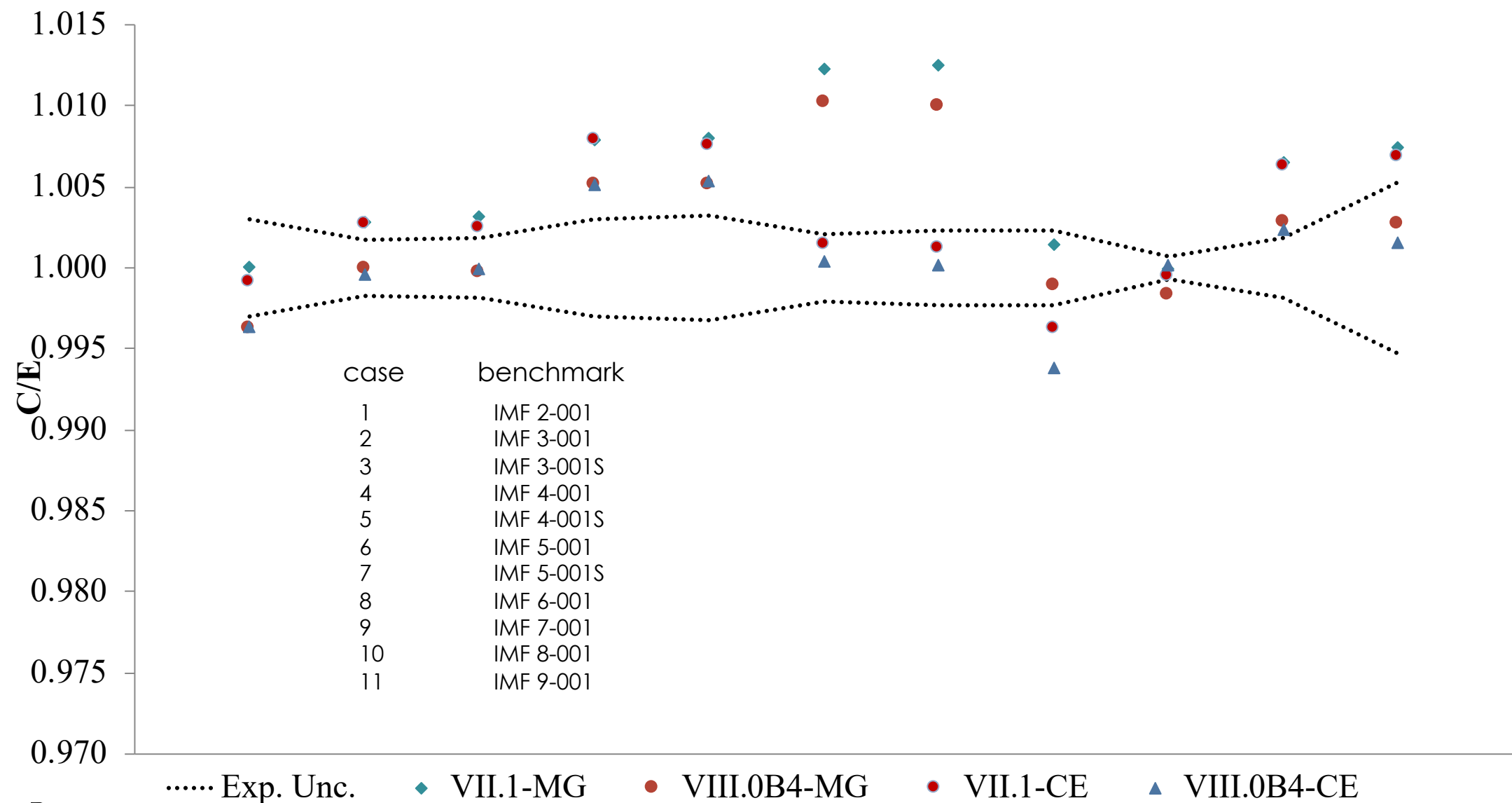
Templates to run the same tests with MCNP are also available (except for thermal moderators).

Ensure that enough particles/generations are run if a direct comparison is desired.

# Test the new library

- Run SCALE cases that are relevant to your problem
- At ORNL we run VALID

# IMF Results from VALID



## Other AMPX functionality

- If you want to use the new library in depletion calculations you will need to generate the JEFF-3.2 activation library in your group structure (use template `origenlib` and `combine_mgs`)
- If you want to make a coupled library, the process is almost the same as shown here, except use additional template `gamma_mg`. Additional SCALE transmission unit tests are available.
- If you want to generate covariance data, use templates `puff` and `combine_cov`.
- Custom templates can be added to ExSite, to for example compare AMPX and NJOY results. Codes that compare libraries are available in AMPX.