OAK RIDGE National Laboratory

Generation of SCALE Multi-Group Libraries with AMPX

Dorothea Wiarda
Andrew Holcomb
Friederike Bostelmann

SCALE USERS' GROUP WORKSHOP
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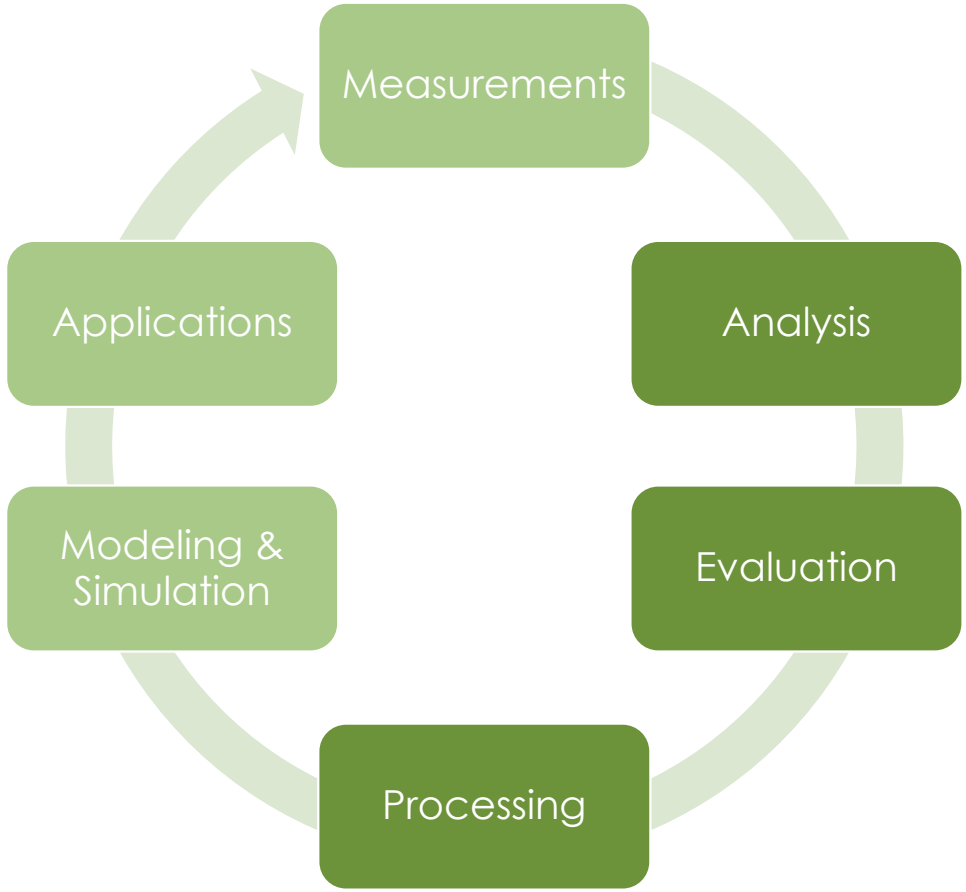
U.S. DEPARTMENT OF ENERGY

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

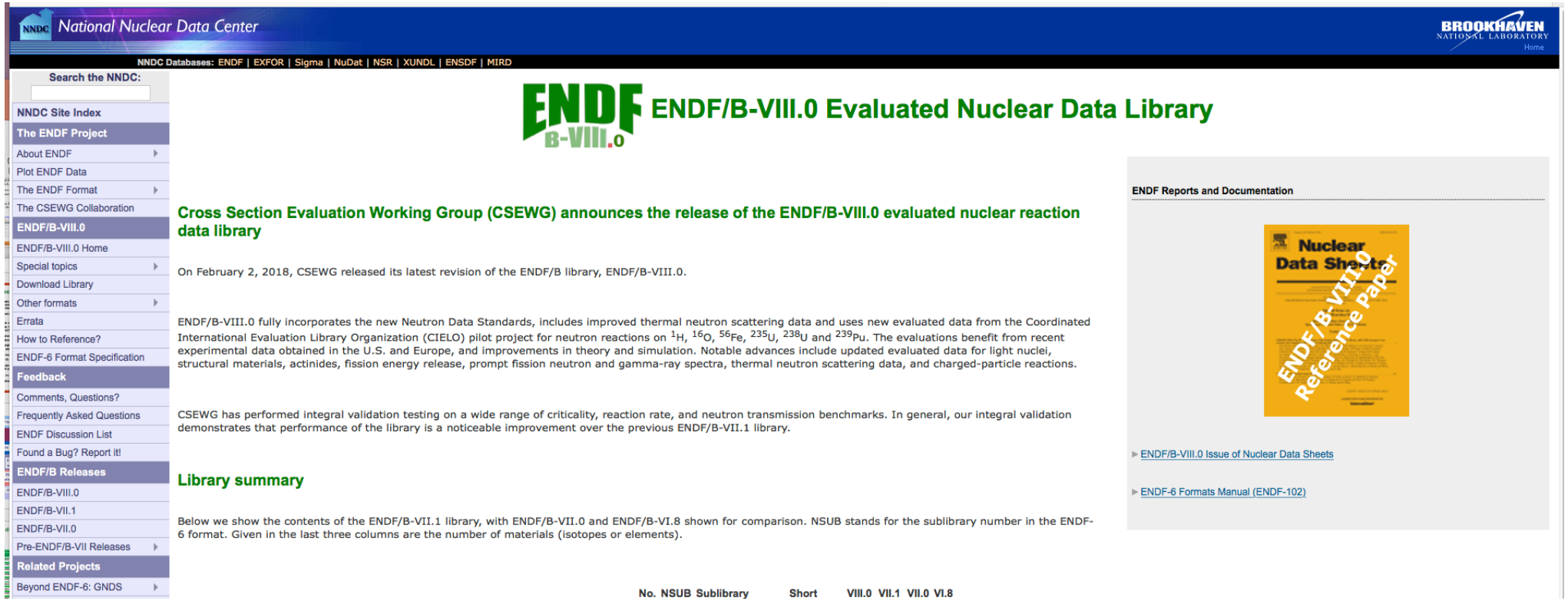
- AMPX processes data in Evaluated Nuclear Data Files (ENDF) to provide CE, MG, Covariance, and ORIGEN Data Libraries for SCALE
- AMPX developed and maintained at ORNL for over 40 years
- 1990: ENDF Formats changed significantly with ENDF/B-VI release in 1990—AMPX could no longer process latest ENDF 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)

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

- 2012 – Present: Modernization effort to implement SQA and modern software design/development practices
- Current version available with SCALE 6.2 and up

How to get data files

- ENDF - http://www.nndc.bnl.gov/endf/b8.0/index.html



- JEFF - https://www.oecd-nea.org/dbdata/jeff/
- JENDL - https://wwwndc.jaea.go.jp/jendl/j40/j40.html
- Other data projects

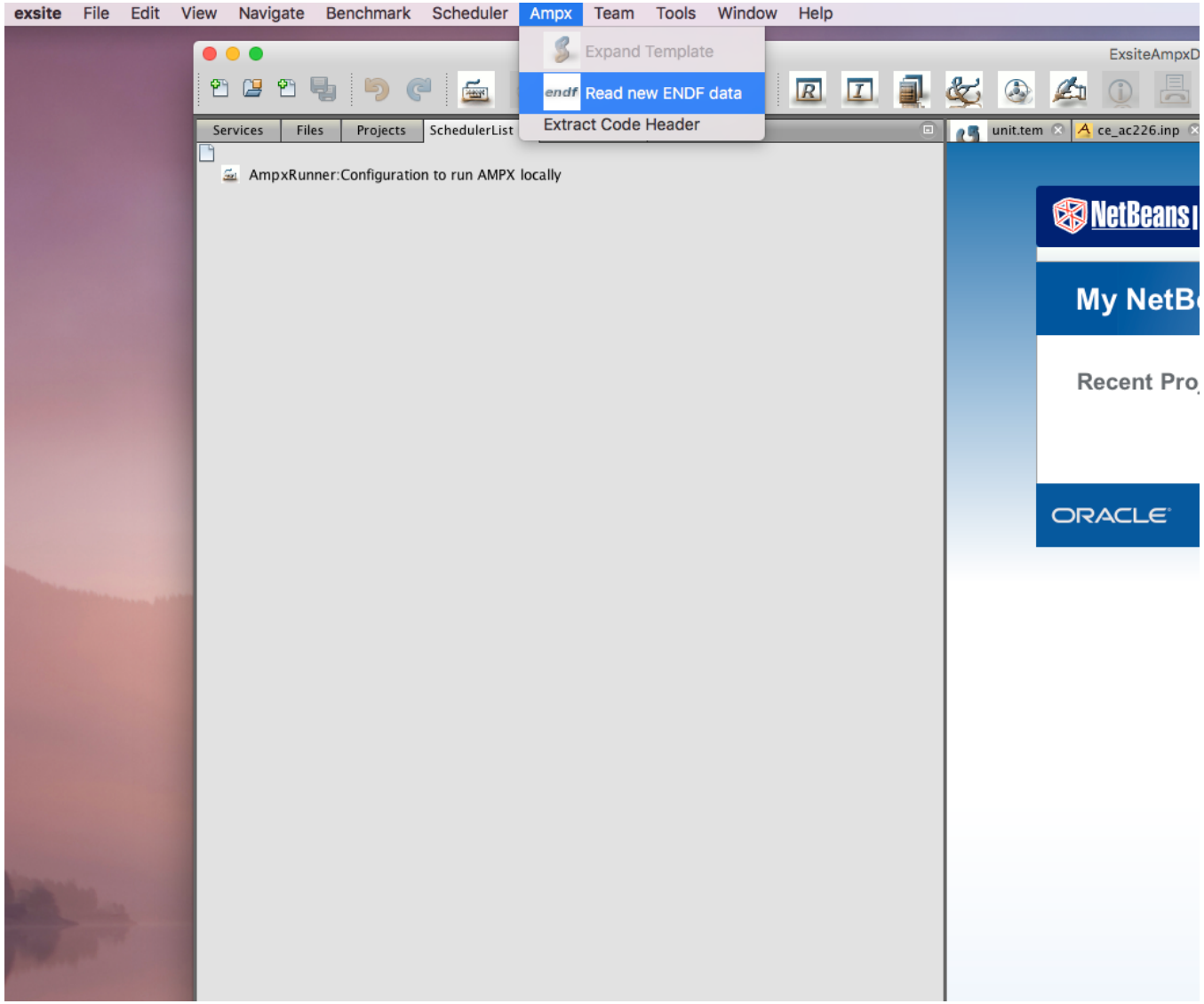
ENDF sub libraries

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	
10	**Neutron**	**n**	**MG/CE libraries**
11	Neutron fis. yields	nfy	Origen library data
12	**Thermal scattering**	**tsl**	**MG/CE libraries**
19	Standards	std	
113	Electro-atomic	e	
10010	Proton	p	
10020	Deuteron	d	
10030	Triton	t	
20030	^{3}He	he3	
20040	^{4}He	he4	

Thermal scattering data

- Thermal scattering data exist in thermal range (<10eV) 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.



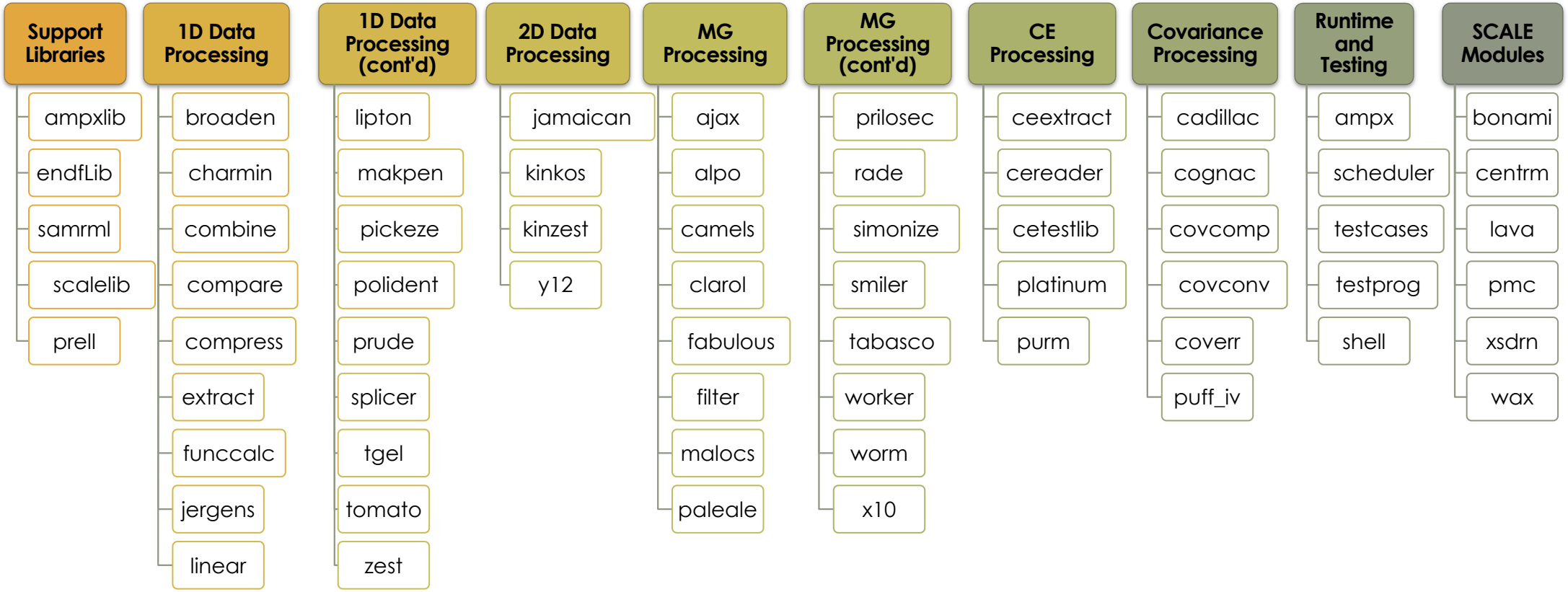
XML ENDF listing

```
<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"
/>
```

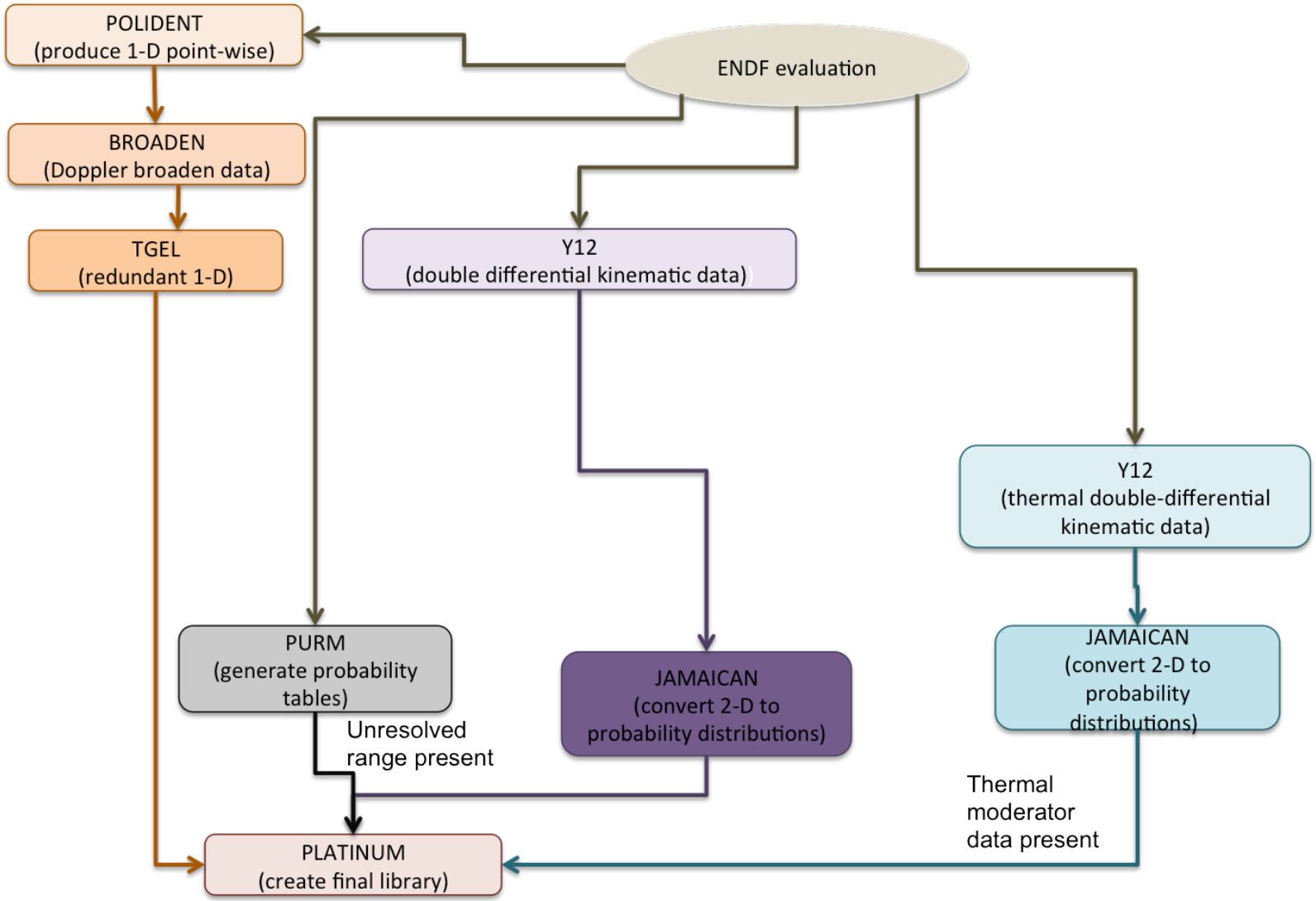
Examine _config file

```
<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>
```

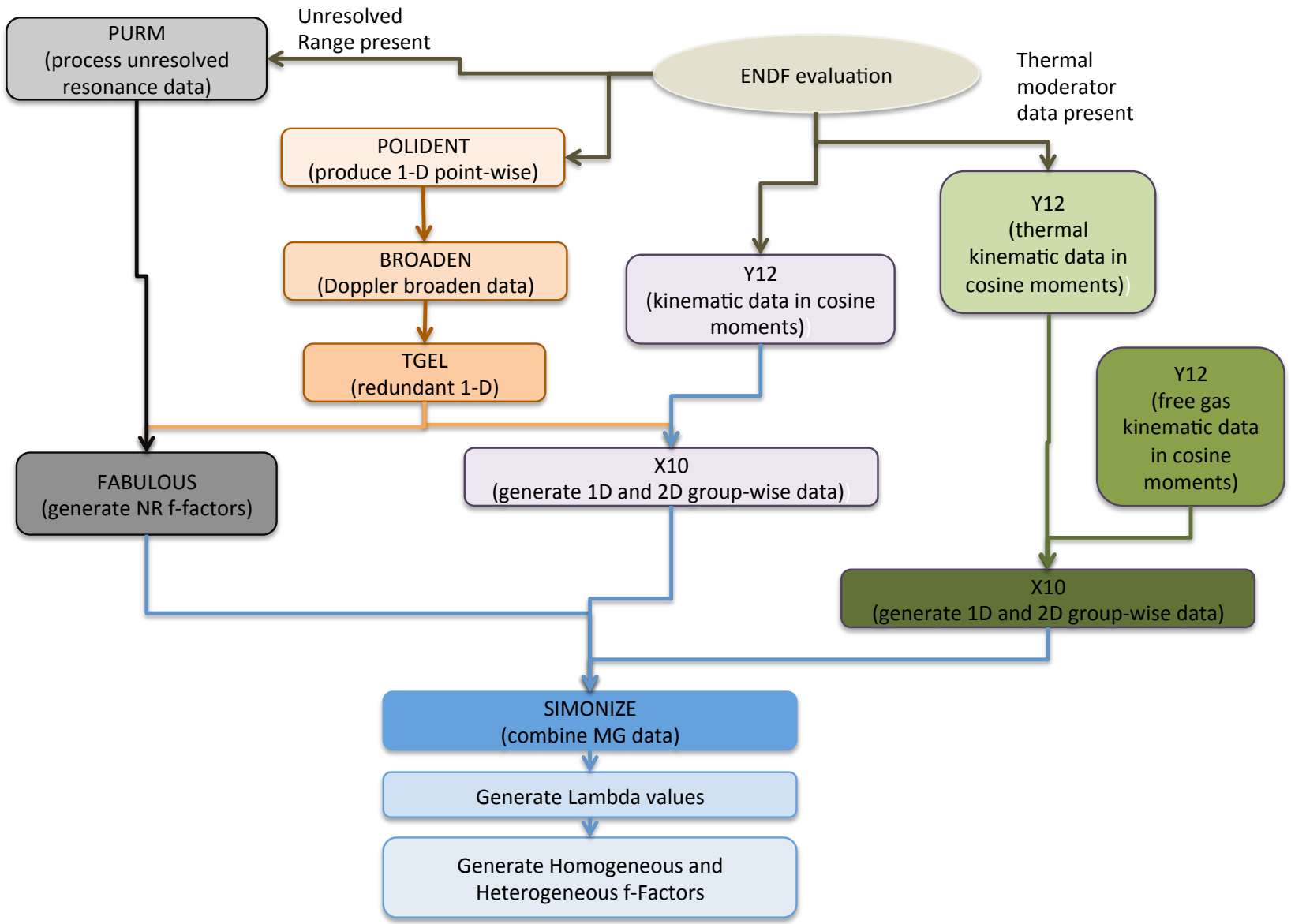
AMPX Modular Code System



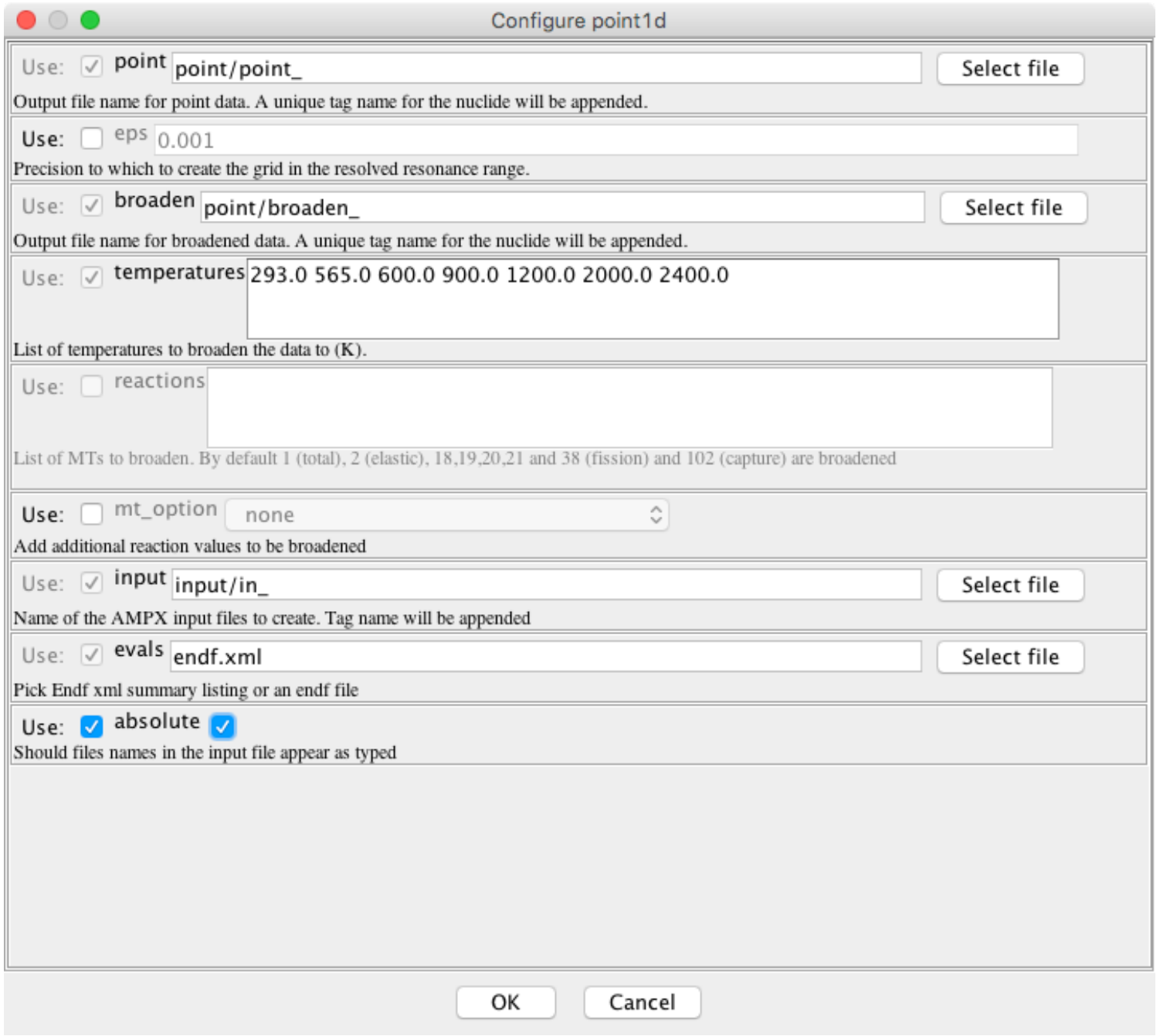
Processing CE Libraries



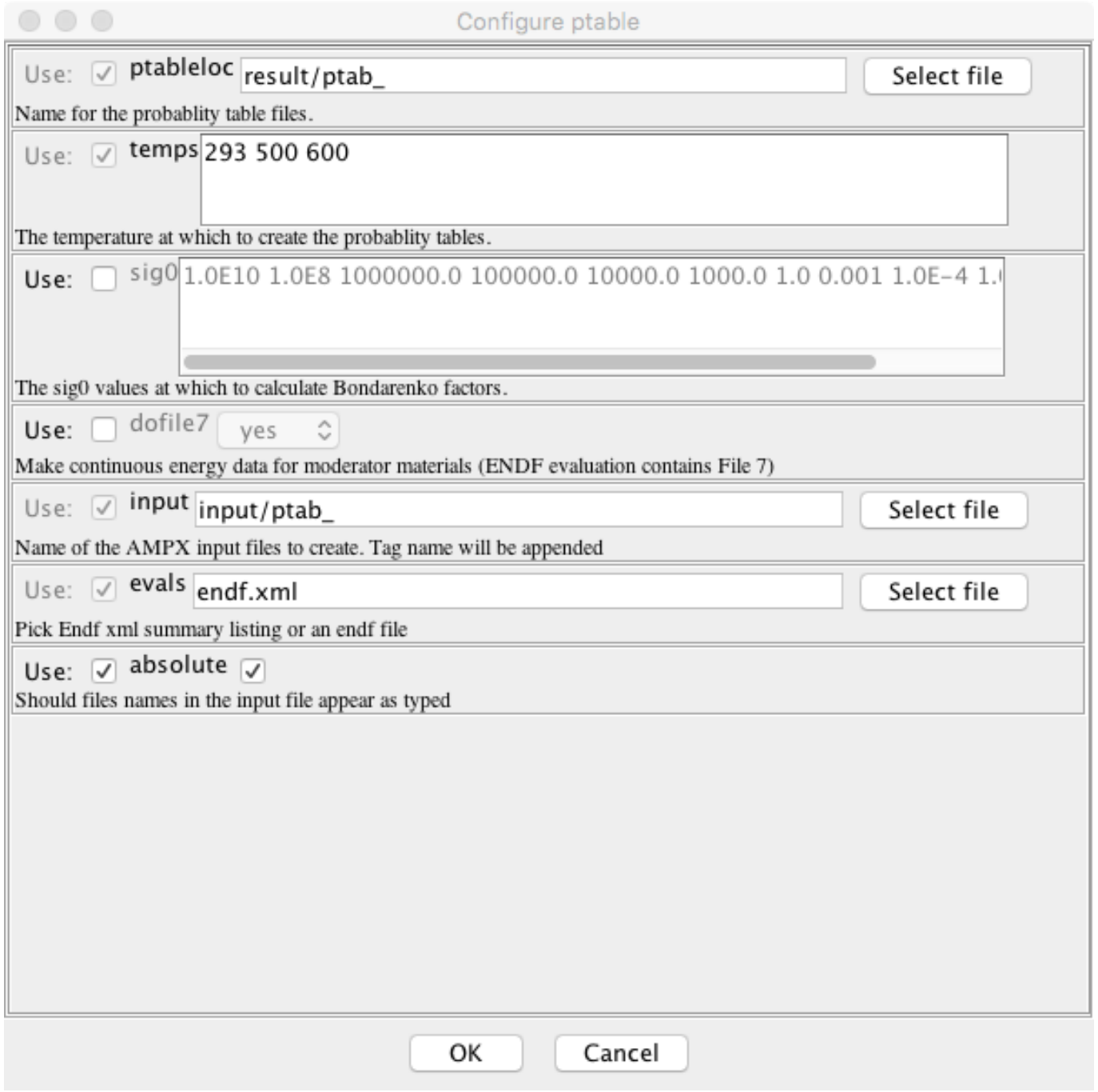
Processing MG Libraries



Point1d expansion

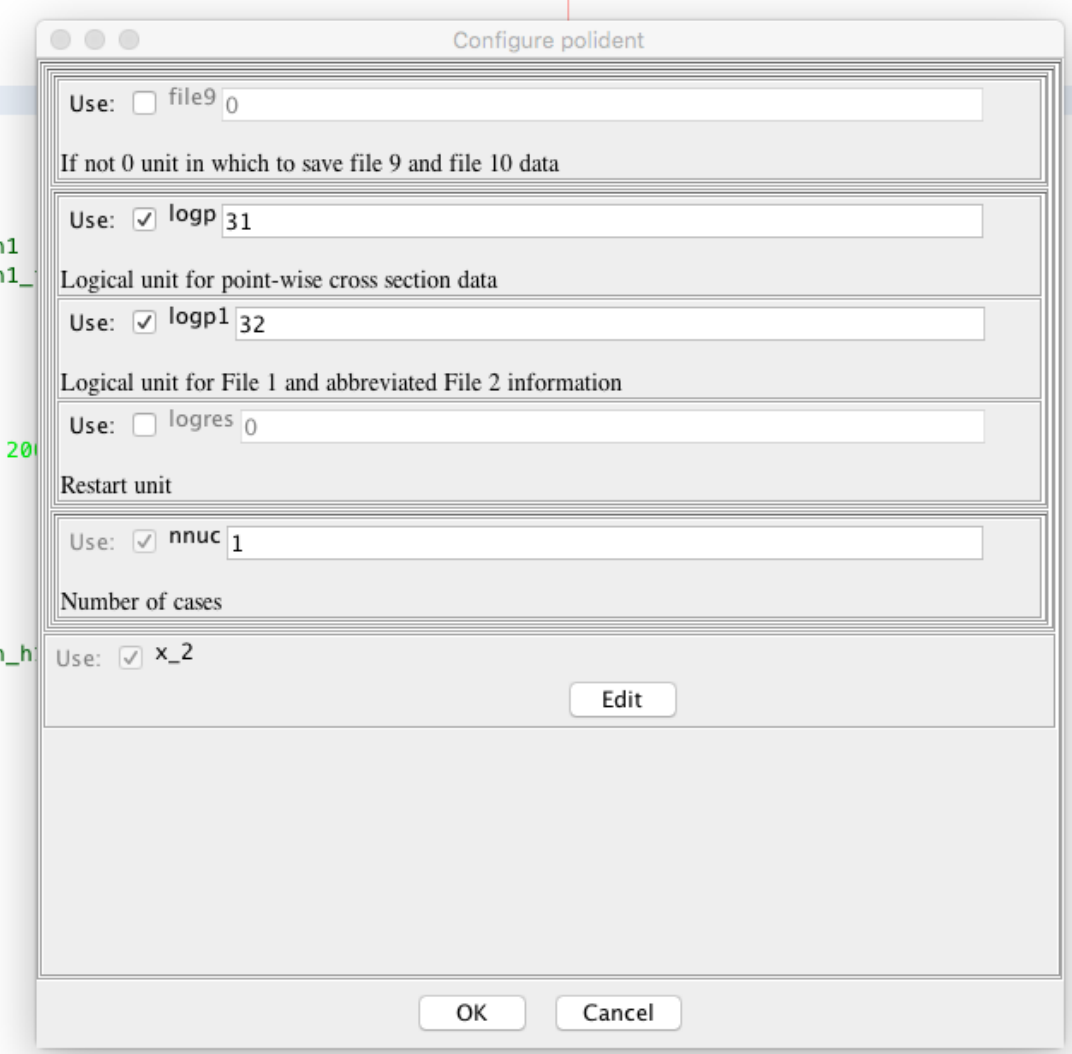


P-table expansion



Examine the input files

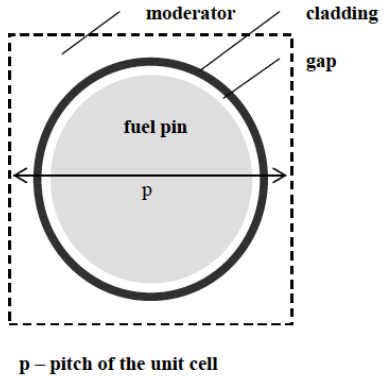
```
=shell
ln -sf /Users/dw8/ampx/endf/svn_endf/endf7/neutrons/n-001_H_001.endf ft11f001
end
=polident
-1$$ 0
0$$ 31 32 e 1$$ 1 t
2$$ 125 11 2 6 e
4** a5 0.001 e
6$$  a3 0 15000 t
end
=shell
cp ft31f001 ${RTNDIR}/../result/point_h1
cp ft32f001 ${RTNDIR}/../result/point_h1_
end
=tgel
input=31 output=33 total
end
=broaden
t= 0.0  293.0 565.0 600.0 900.0 1200.0 20
logpt=33 logdp=34
end
=tgel
input=34 output=35 total
end
=shell
cp ft35f001 ${RTNDIR}/../result/broaden_h
end
```



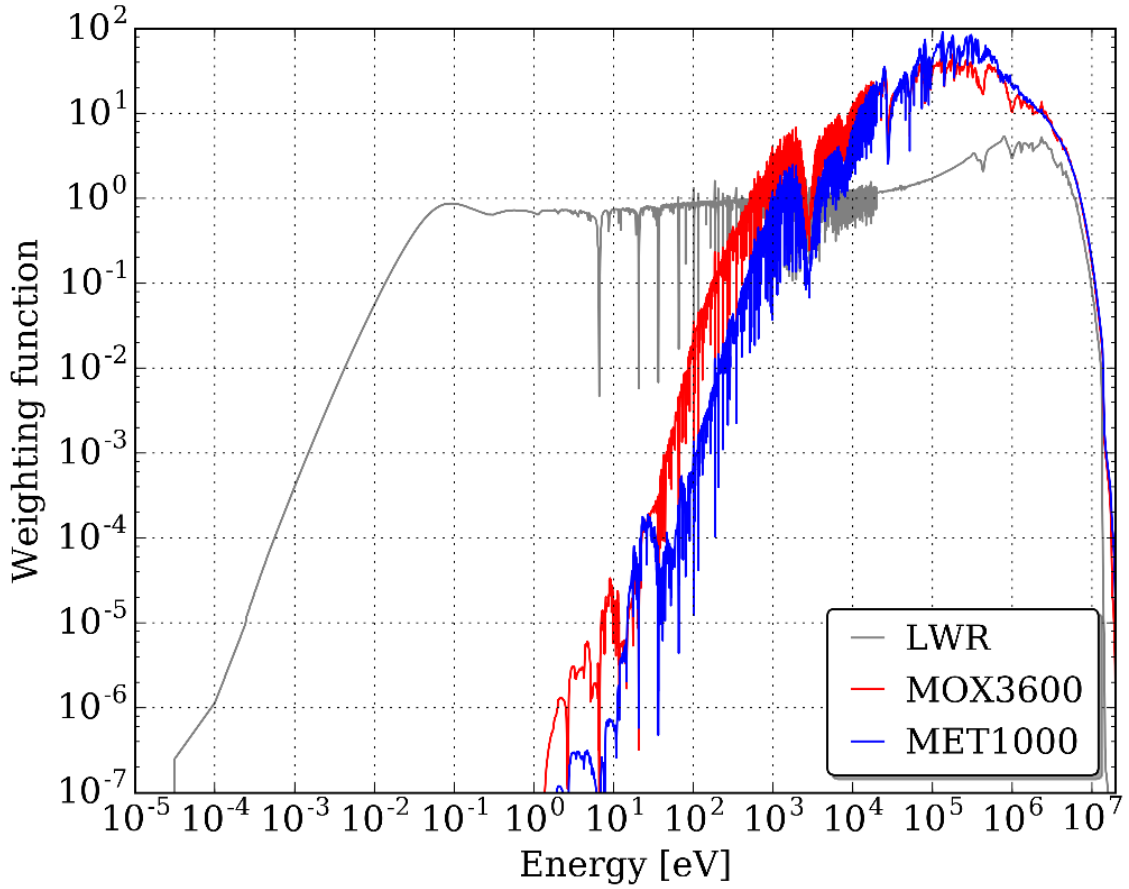
Flux selection

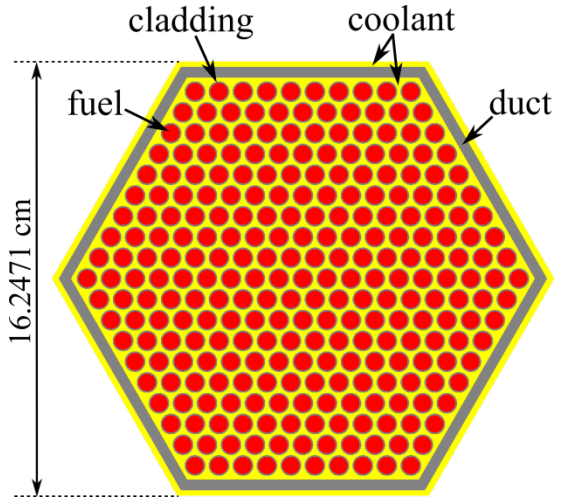
- Flux is just a 1-D function over Energy in eV.
- Any 1-D function can be used (there are programs that convert to ASCII (x,y) values to the needed binary file.
- Flux can be temperature and ZA dependent.
- Flux can be generated from a CENTRM run.
- For the tutorial we are using the standard weighting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

Flux choices

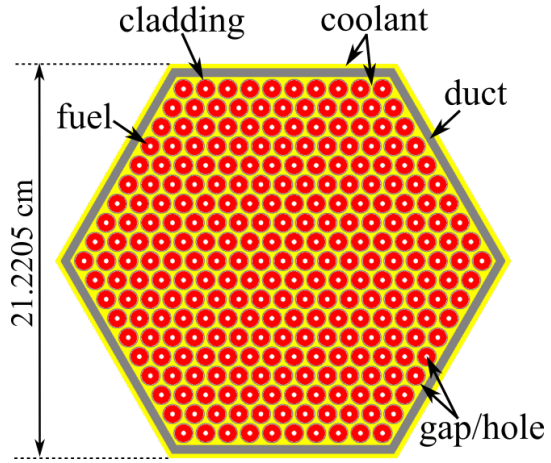


LWR pin cell





MET1000 fuel assembly



MOX3600 fuel assembly

*Figure: NEA/NSC/DOC(2013)7, May 2013.

Homogenized SFR fuel assembly

MG library	k_∞	$\Delta\rho = (1/k_{ref} - 1/k_\infty)$ [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)**

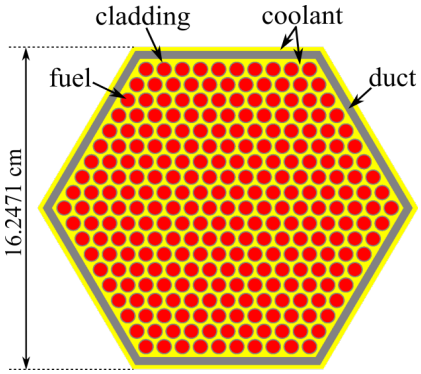
252g LWR:
- group structure optimized for thermal systems
- weighting function LWR spectrum
- SCALE standard library

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

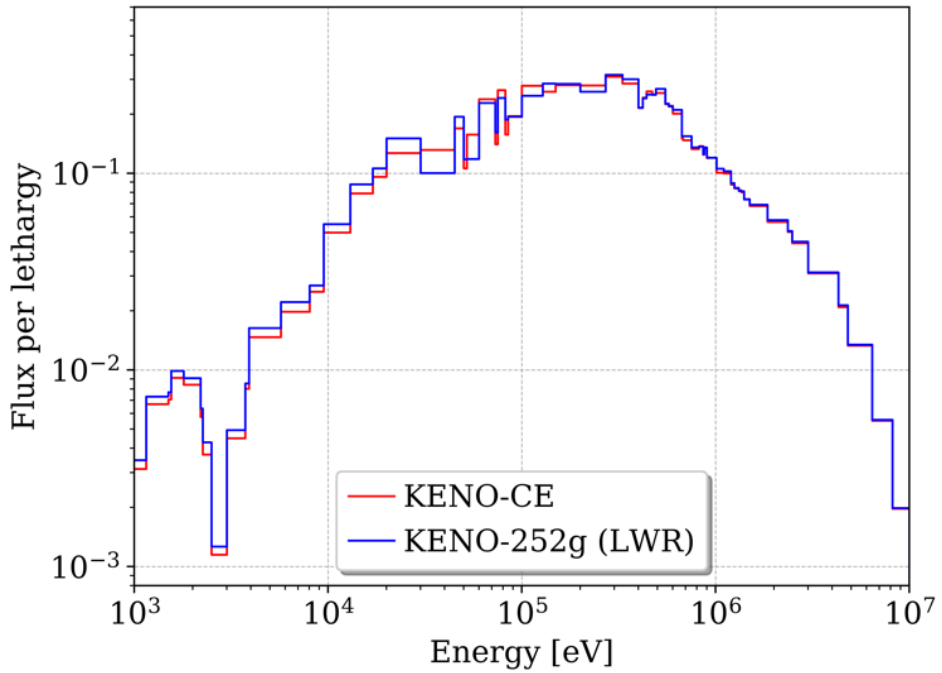
Influence of weighting spectrum

Influence of energy group structure

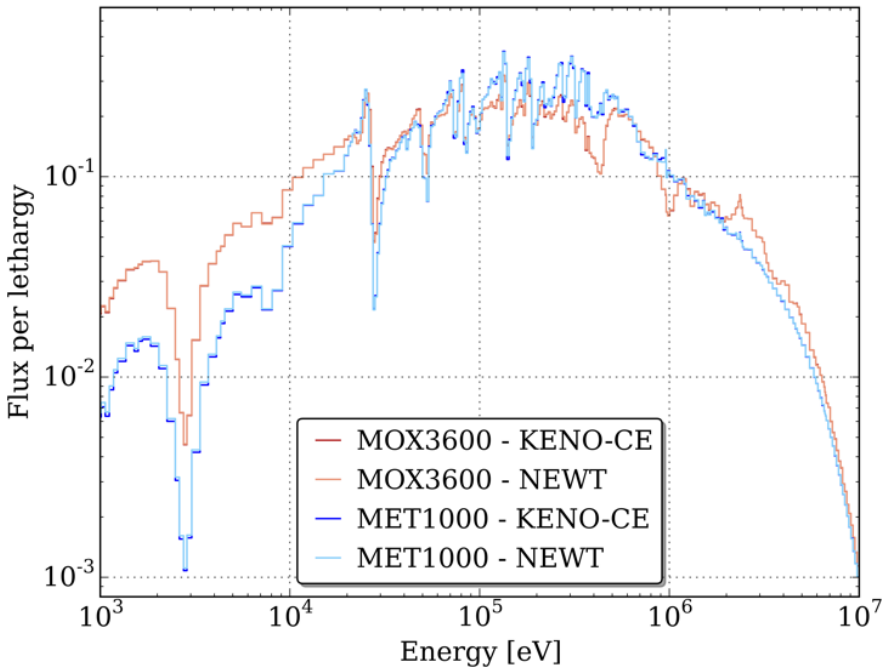
Neutron flux of a homogenized SFR fuel assembly



MET1000



KENO 252g calculation



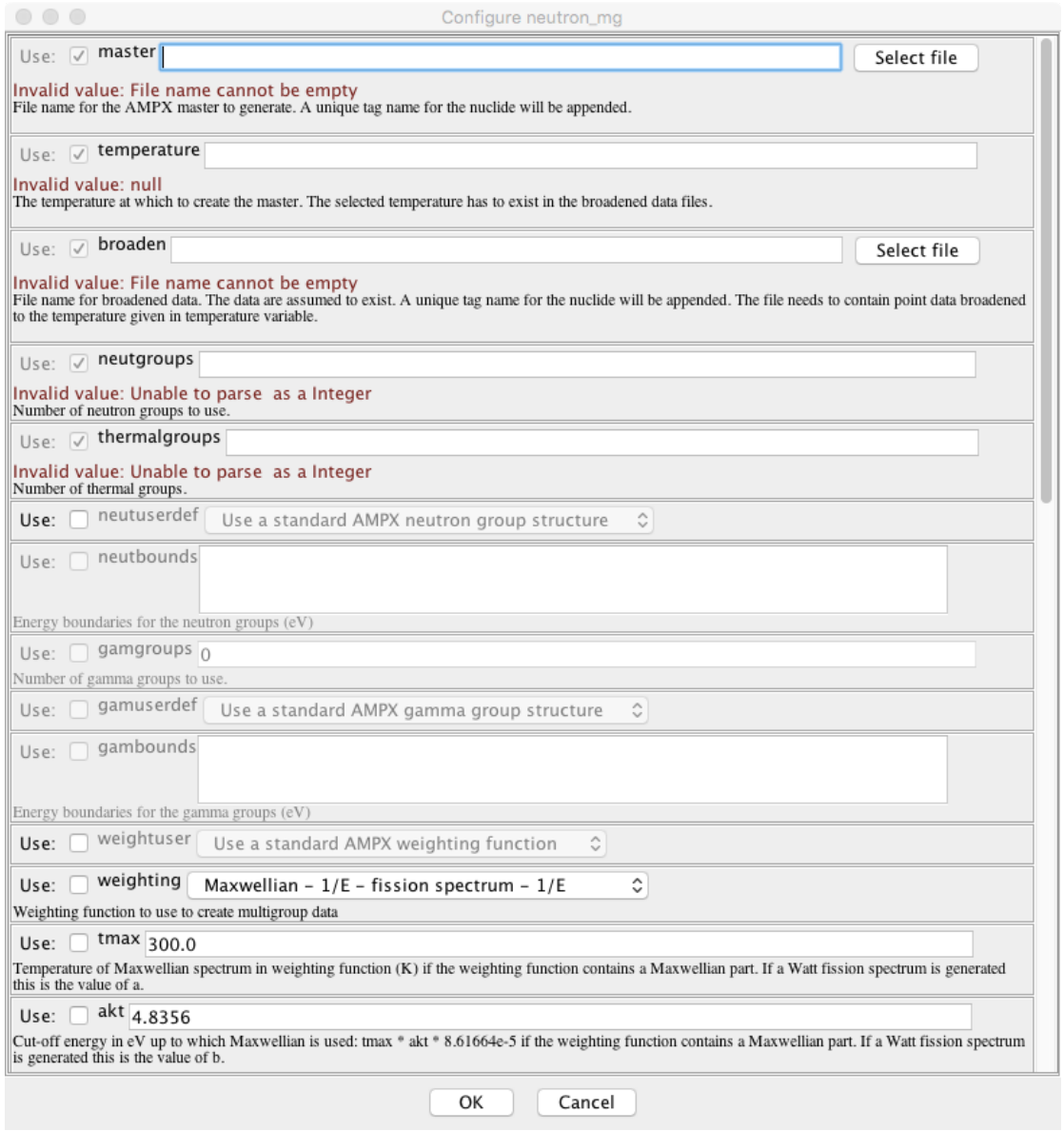
KENO 302g (SFR) calculation

Some VALID calculations

Experiment	Measurement	CE	252g	302g	Δk (252g vs. CE) [pcm]	Δk (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



Bondarenko Factors

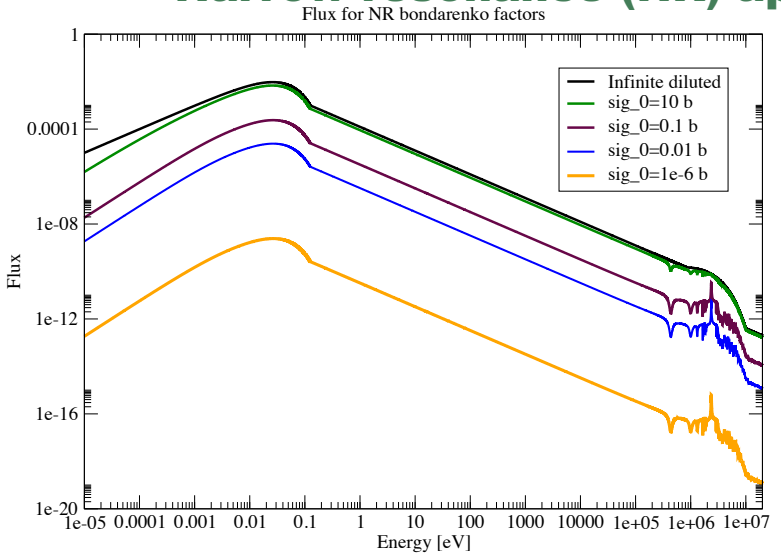
Calculate problem independent cross section data as a function of background cross section and temperature:

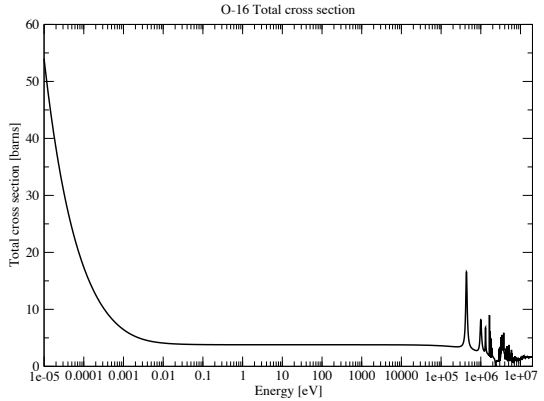
$$\sigma_{x,g}^{(j)}(\sigma_0,T)=\frac{\int_g \sigma_x^{(j)}(E,T)\,\varphi(E,\sigma_0,T)\,\mathrm{dE}}{\int_g \varphi(E,\sigma_0,T)\,\mathrm{dE}}$$

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





Flux for ^{16}O for different background values

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

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

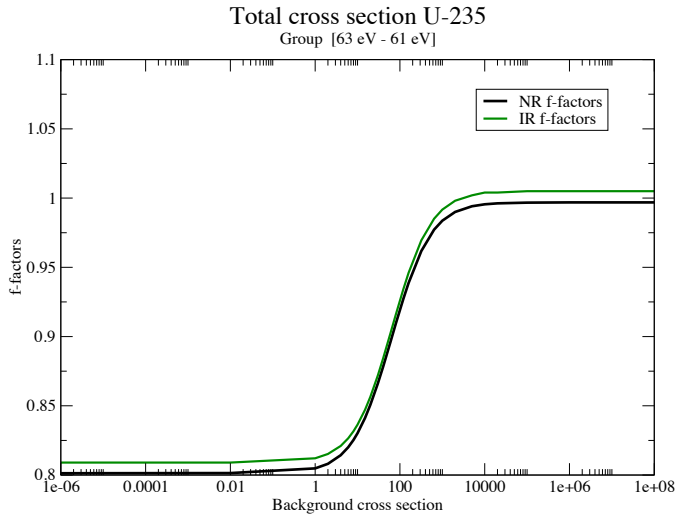
$$\left(\sigma_t^{(j)}(E,T)+\sigma_0\right)\varphi(\mathrm{E},\sigma_0,T)=\int_E^{E/\alpha^{(j)}}\frac{\sigma_s^{(j)}(E',\mathrm{T})\varphi(E',\sigma_0,\mathrm{T})}{(1-\alpha^{(j)})E'}dE'+\sigma_0\int_E^{\infty}\frac{\varphi(E',\sigma_0\,\mathrm{T})}{E'}dE'$$

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

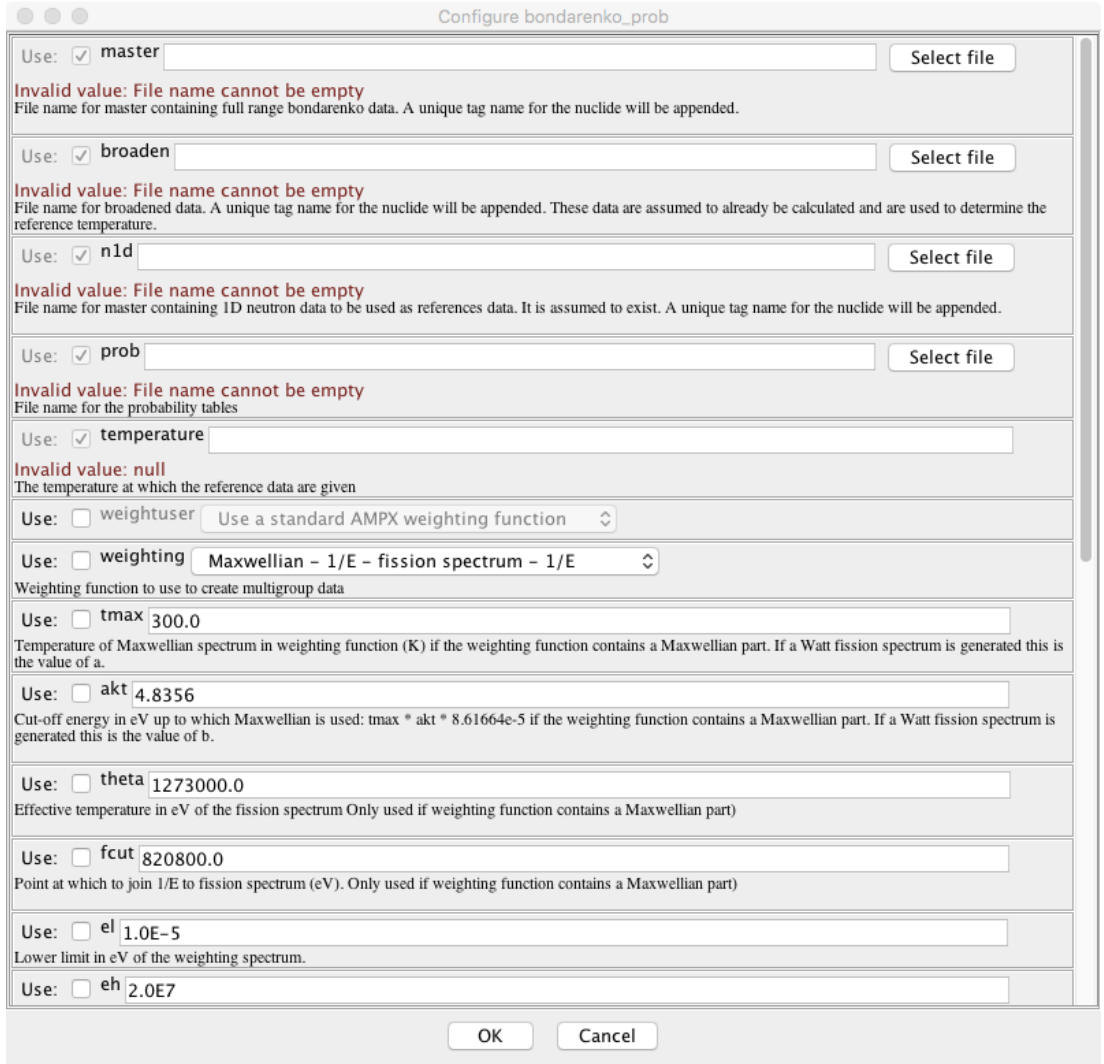
$\sigma_0=\frac{N^{(H)}}{N^{(j)}}\sigma_p^{(H)}$ (the background cross section);

$\sigma_p^{(H)}$ = 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



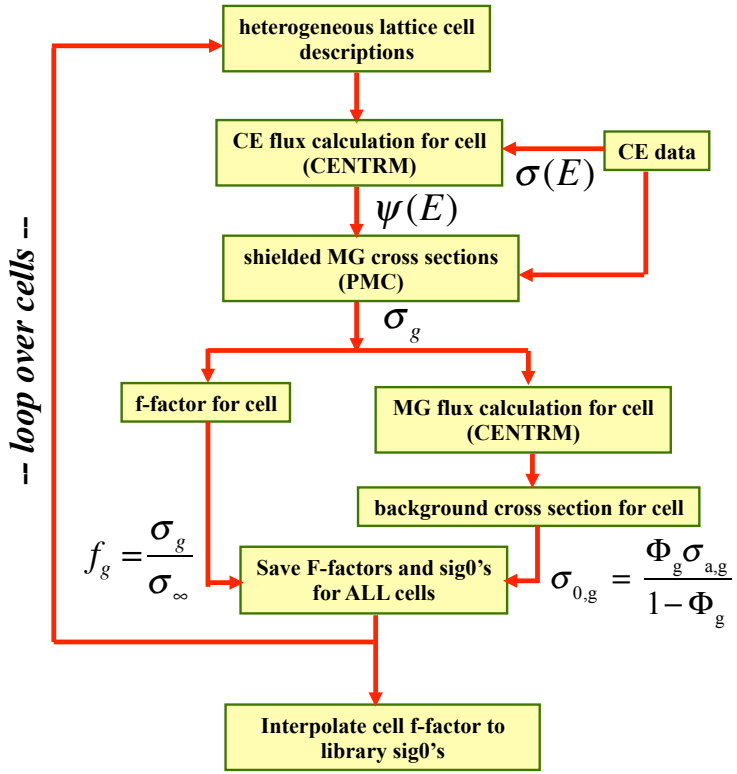
Bondarenko template



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

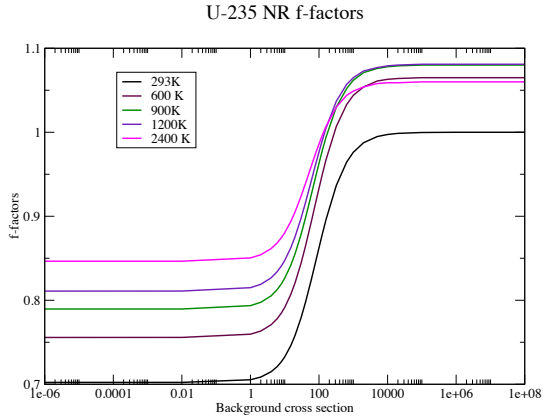
In order to account better for in-group elastic scattering, f-factors (NR and IR) can be added to a MG library.

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.



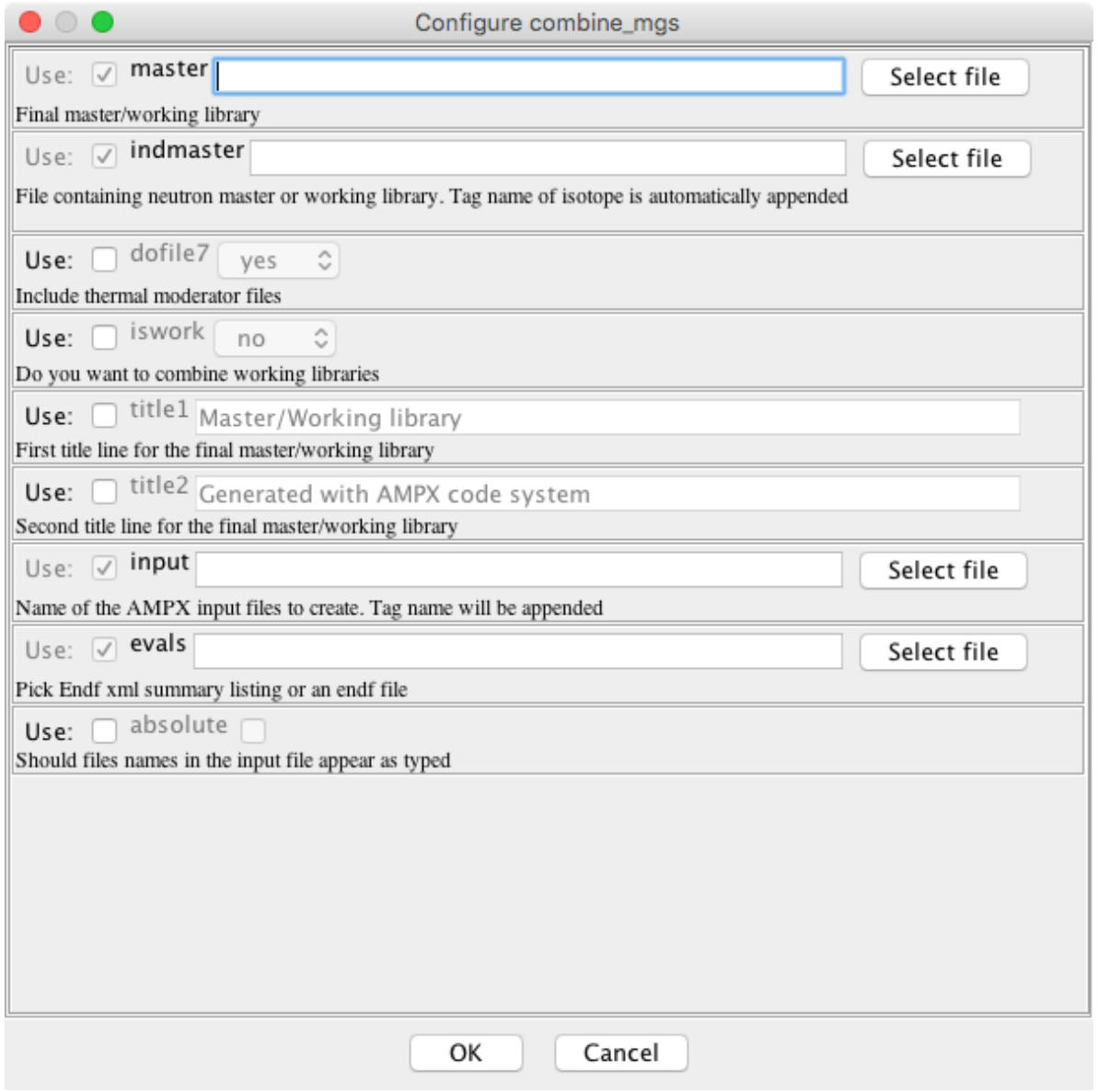
209.5 eV – 207.4 eV

Bind the library for each nuclide

Start Page | test.tem | bind_h_h2o_thermal.inp

```
=shell
ln -sf  ${RTNDIR}/../result/neut__neutron_h1  ft01f001
ln -sf ${RTNDIR}/../result/bond_h_h2o_h1 ft03f001
cp ft03f001 ft33f001
ln -fs ${RTNDIR}/../result/neut_h_h2o_thermal_1001 ft04f001
end
=filter
in=4 out=44 1dn mt=1007 1008
end
=simonize
Identifier=1001 master=20
title= h_h2o 1 fast: h1 endf-8 REL0 REV8 MOD0
za=10010
fastid=8000125 thermid=8000001 source=0 BONDARENKO=3 id19=125
1dn=33 id19=125
2dn=4 id19=1001 MT=0 MODERATOR
1dn=44 id19=1001

neutron=1 id19=125
end

=ajax
0$$ 21 e 1$$ 1 t
2$$ 20 0 e t
h_h2o 1 fast: h1 endf-8 REL0 REV8 MOD0
end
=rade
1$$ 21 e t
end
=shell
cp ft21f001 ${RTNDIR}/../result/master_h_h2o_h1
end

```

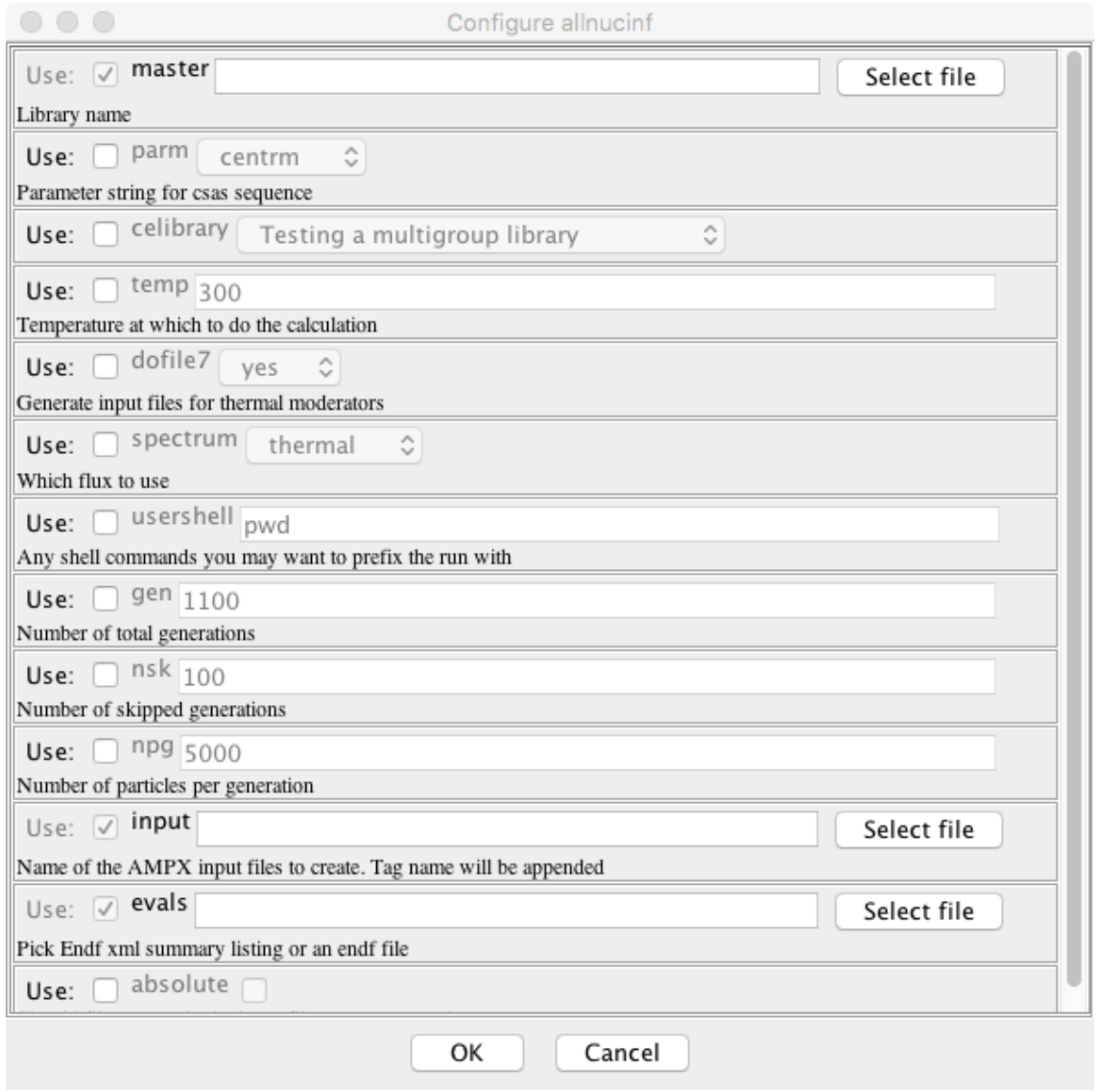
Make an AMPX master library



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



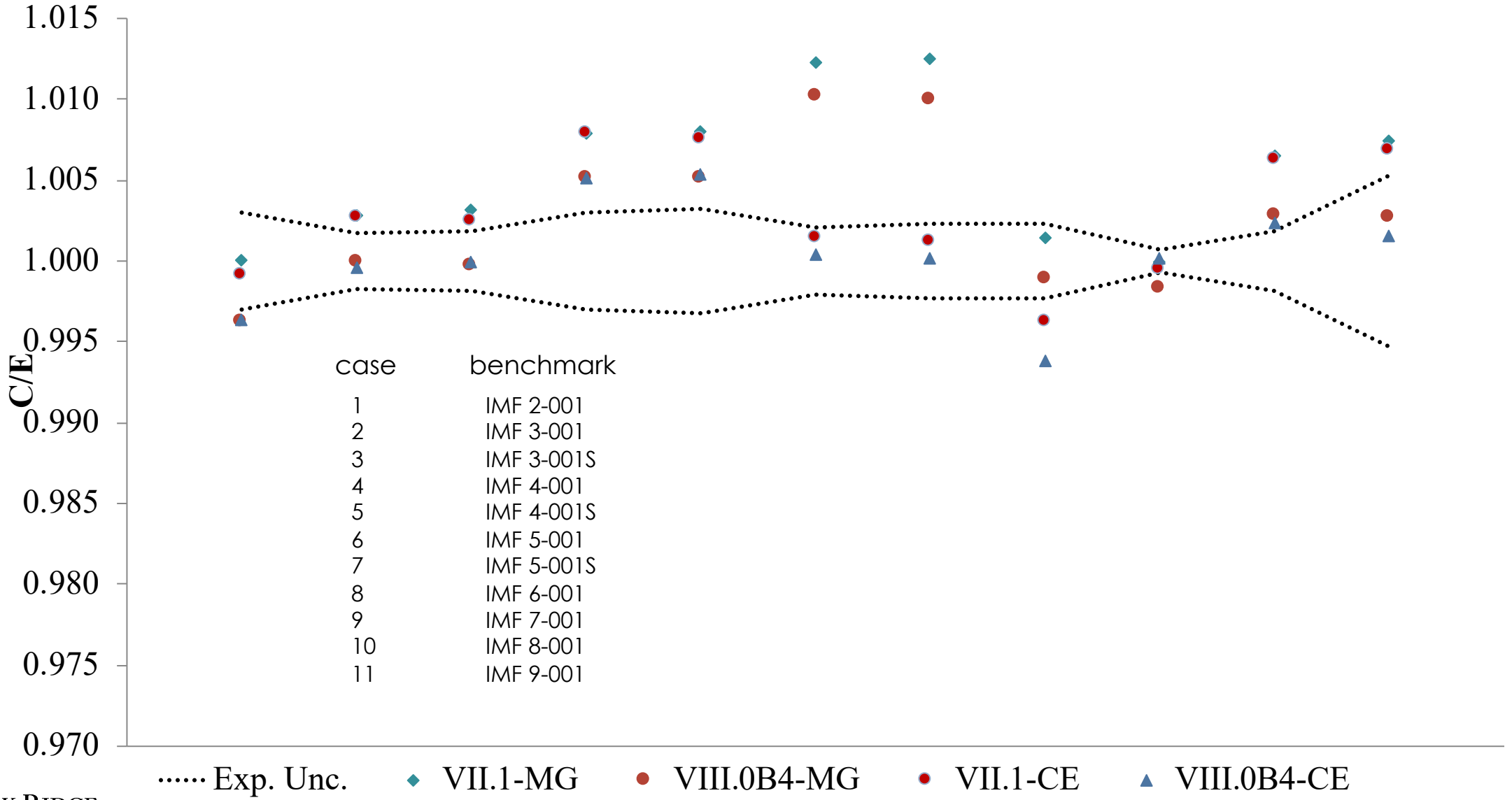
Templates to run the same tests with MCNP are also available (except for thermal moderators).

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.