POLYTECHNIQUE
MONTRÉAL

Production of multigroup nuclear data libraries

A. Hébert

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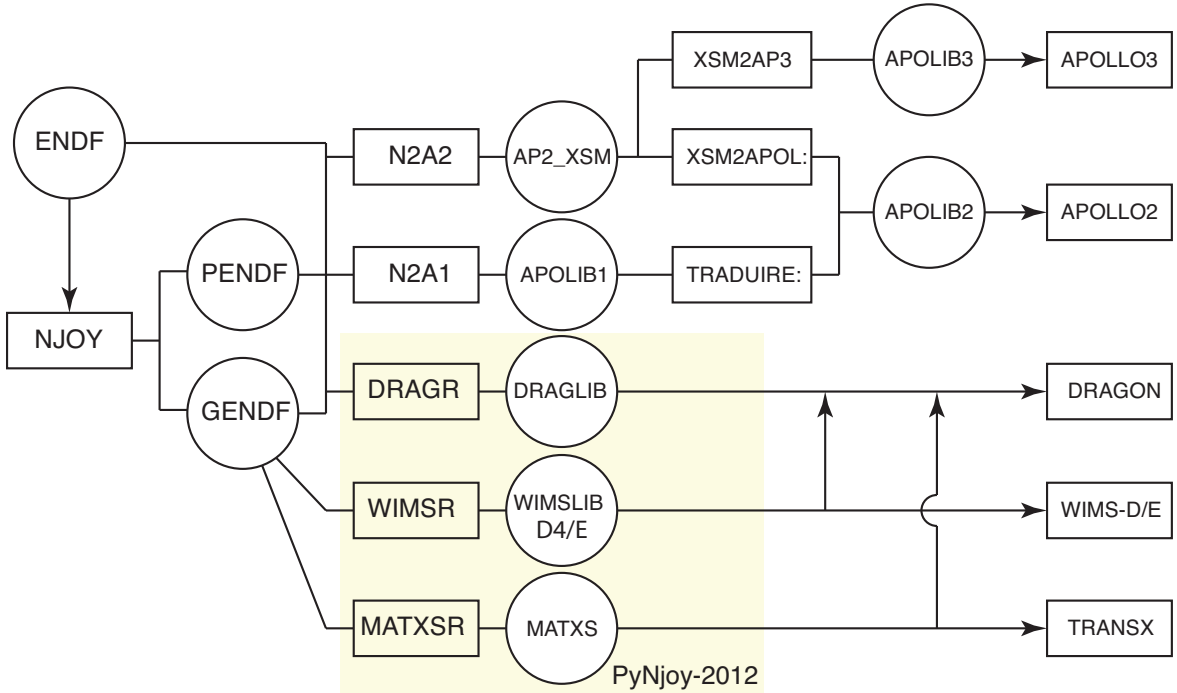
General presentation

Multigroup nuclear data libraries are required as input to lattice codes:



- The SCIENCE system for Pressurized Water Reactors (PWR) is based on APOLLO2 lattice code.
- The PyNjoy-2012 system developed at EPM is currently used to produce libraries in DRAGLIB and WIMSLIB-E formats.

The PyNjoy 2012 system

The NJOY saga NJOY is the official Los-Alamos software for processing nuclear data evaluations in the ENDF format.

NJOY-99 The last distribution of the code written in Fortran-77.

NJOY-2012 A major rewrite of the code written in Fortran-90.

- Still based on UPD system for implementing updates.
- Los-Alamos license.
- Used by DRAGON, CASMO, WIMS, MONK, APOLLO, ERANOS and SCALE.

NJOY-2016 Equivalent to NJOY-2012, without UPD.

- Based on GIT for source update
- Open source

NJOY-2021 A major rewrite of the code written in C++.

- Can process evaluations in Generalized Nuclear Data (GND) format in addition to traditional ENDF-102 format
- Open source

The PyNjoy 2012 system

The PyNjoy 2012 system is made of the following components:

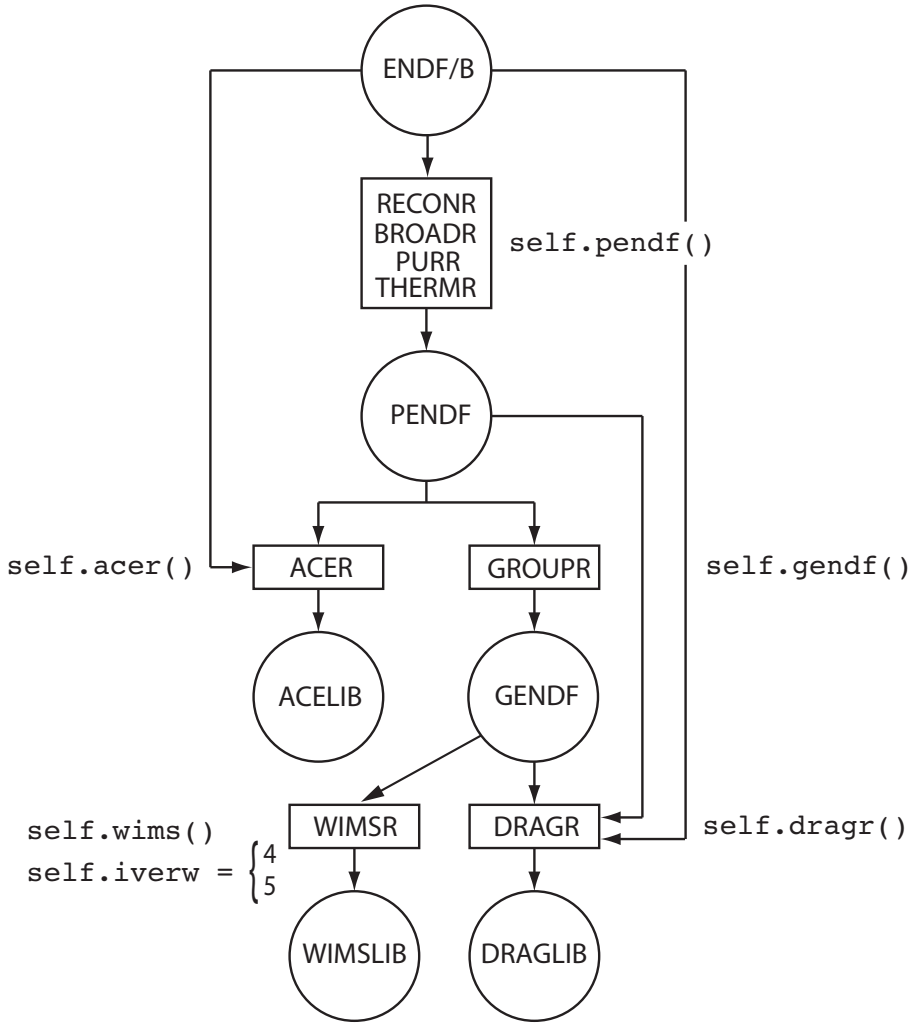
1. The NJOY-2012.0 distribution, as released by LANL.
2. A new Fortran-2003 module named `dragr` and included in the NJOY-2012 source for processing ENDF, PENDF and GENDF files and for producing the output DRAGLIB file.
3. New NJOY-2012 updates from EPM. These updates contain bug fixes and additional energy meshes for the `groupr` module:

   SHEM-281: Santamarina-Hfaiedh 281-group energy mesh used at the CEA, Areva, and EDF.
   SHEM-361: 361-group energy mesh defined as a collaboration between the CEA and EPM.
   SHEM-295: 295-group energy mesh defined at EPM.
   SHEM-315: 315-group energy mesh defined at EPM.
   Rahab-89: 89-group energy mesh defined at Atomic Energy of Canada Limited (AECL).

4. A generic Python script named PyNjoy.py for automating the preparation of datasets for NJOY. Processing of complete ENDF evaluations is greatly facilitated with the help of this script. The script is used for processing isotopes and for constructing depletion chains.
5. A collection of Python datasets, each of them corresponding to a specific evaluation (Jeff3.1, ENDFB-VII rel. 0, etc.) processed with a specific multigroup energy mesh (XMAS-172, SHEM-281, etc.).

The PyNjoy 2012 system

The flowchart of NJOY-2012 processing, including `dragr`, is presented here:



The dragr module

The DRAGR module was written as a clean and direct utility to format a DRAGLIB library, using PENDF and GENDF data.

- Care was taken to avoid unnecessary processing of nuclear data and to keep the richness of ENDF/B information.
- Other advantages are related to the use of the DRAGLIB format, thanks to the careful design of its direct access procedure.
- The cross-section processing in DRAGR is similar to the approach used in module MATXSR.
- The library file can be converted back and forth between a sequential ASCII format and a binary direct access format. DRAGR contains all management capabilities built-in. There is no need to use any auxiliary program such as BCD.

The dragr module

Cross-section information

- The steady-state fission spectrum, $\chi(g)$, is assumed to be dilution independent. It is calculated using

$$\chi(g) = \frac{\sum_h \sigma_f(g \leftarrow h)\phi_0(h)}{\sum_g \sum_h \sigma_f(g \leftarrow h)\phi_0(h)} \tag{1}$$

  where $\sigma_f(g \leftarrow h)$ and $\phi_0(h)$, the library weight function for the first Legendre order, are recovered from `MF=6` and `MT=18` records of the GENDF file.
- The steady-state $\nu\sigma_f$ values are calculated using

$$\nu\sigma_f(g) = \sum_h \sigma_f(h \leftarrow g) \ . \tag{2}$$

The dragr module

- The delayed fission spectra, $\chi_\ell^{\text{del}}(g)$, are assumed to be dilution independent. They are calculated using

$$\chi_\ell^{\text{del}}(g) = \frac{\nu_\ell^{\text{del}}(g)}{\sum_h \nu_\ell^{\text{del}}(h)} \tag{3}$$

  where $\nu_\ell^{\text{del}}(g)$ is recovered from `MF=5` and `MT=455` record of the GENDF file.
- The delayed $\nu\sigma_{\text{f}}$ values are calculated using

$$\nu^{\text{del}}\sigma_{\text{f},\ell}(g) = \pi(g)\left(\sum_h \nu_\ell^{\text{del}}(h)\right)\sigma_{\text{f}}(g) \tag{4}$$

  where $\pi(g)$ is recovered from `MF=3` and `MT=455` record of the GENDF file and $\sigma_{\text{f}}(g)$ is recovered from `MF=3` and `MT=18` record of the GENDF file.

The dragr module

- The scattering matrix for the first Legendre order, $\sigma_{\text{scat0}}(h \leftarrow g)$, describes the energy transfer that follows an isotropic collision in the laboratory system. The collision can be an elastic or inelastic diffusion, a (n,2n), or a (n,3n) reaction. It is calculated from GENDF file information, using

$$\sigma_{\text{scat0}}(h \leftarrow g) = \sigma_{\text{diffusion}}(h \leftarrow g) + \sigma_{\text{n,2n}}(h \leftarrow g) + \sigma_{\text{n,3n}}(h \leftarrow g) \quad (5)$$

This matrix is stored using the sparse storage scheme of the MATXS format, with the help of two h-indexed vectors:

$i_{\text{scat0}}(h)$ = most thermal group index that can produce a secondary n group h;

$n_{\text{scat0}}(h)$ = number of primary groups that can produce a secondary n group h.

The scattering matrices for subsequent Legendre orders are stored in a similar manner. No transport-corrected data is written in the DRAGLIB file; the task of transport correction is handled in the lattice code.

The dragr module

- The thermal cross sections and scattering matrices depend upon the binding between the atoms of the material. They are based on the $S(\alpha,\beta)$ model.
  - Binding effects are taken into account in the $S(\alpha,\beta)$ model for moderating nuclides (H in H_2O, D in D_2O, C in graphite, etc.)
  - A free-gas approximation is used for other nuclides
- The (n,2n) and (n,3n) cross sections are edited from the GENDF file using

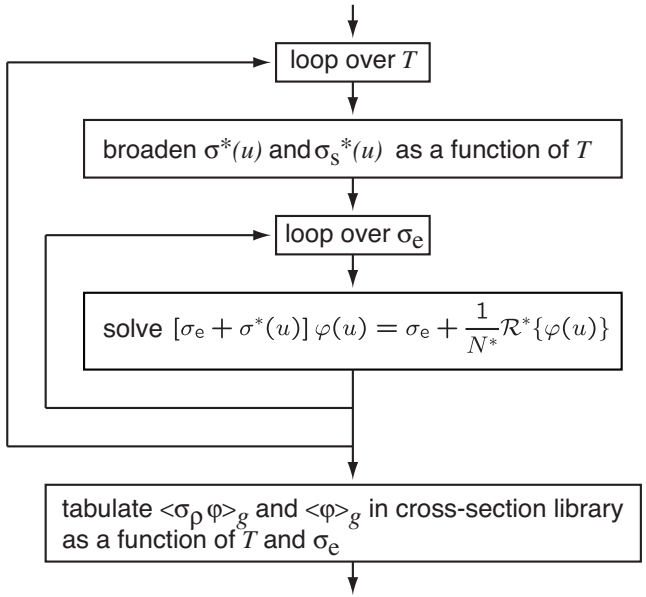
$$\sigma_{\mathrm{n,2n}}(g) = \frac{1}{2}\sum_k \sigma_{\mathrm{n,2n}}(k \leftarrow g) \tag{6}$$

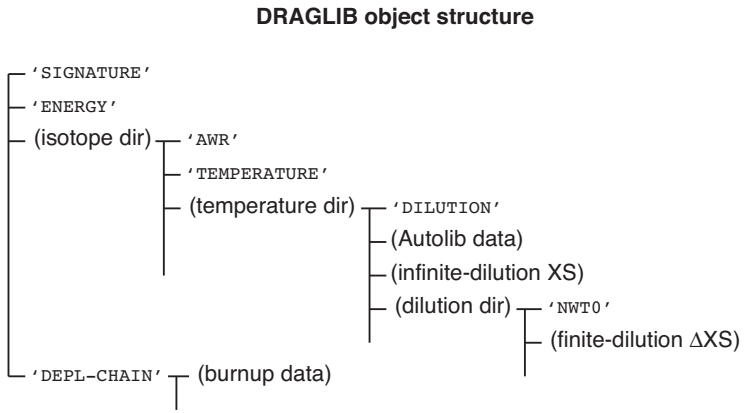
$$\sigma_{\mathrm{n,3n}}(g) = \frac{1}{3}\sum_k \sigma_{\mathrm{n,3n}}(k \leftarrow g) \tag{7}$$

The dragr module

Resonance self-shielding information

- Dilution-dependent information (obtained using the `groupr` flux calculator) is stored on different temperature sub-directories:





- Nuclear data stored on temperature sub-directory is infinite dilution data related to a single isotope at a single temperature.
- Nuclear data stored on dilution sub-directory and corresponding to dilution σ_e is incremental data relative to infinite dilution data.

The dragr module

- ΔXS and $\delta\varphi$ data for each finite dilution σ_e is defined as

$$\delta\sigma_{\mathrm{x}}(g,\sigma_e) = I_{\mathrm{x}}(g,\sigma_e) - \sigma_{\mathrm{x}}(g,\infty) = \sigma_{\mathrm{x}}(g,\sigma_e)\varphi(g,\sigma_e) - \sigma_{\mathrm{x}}(g,\infty) \quad (8)$$

and

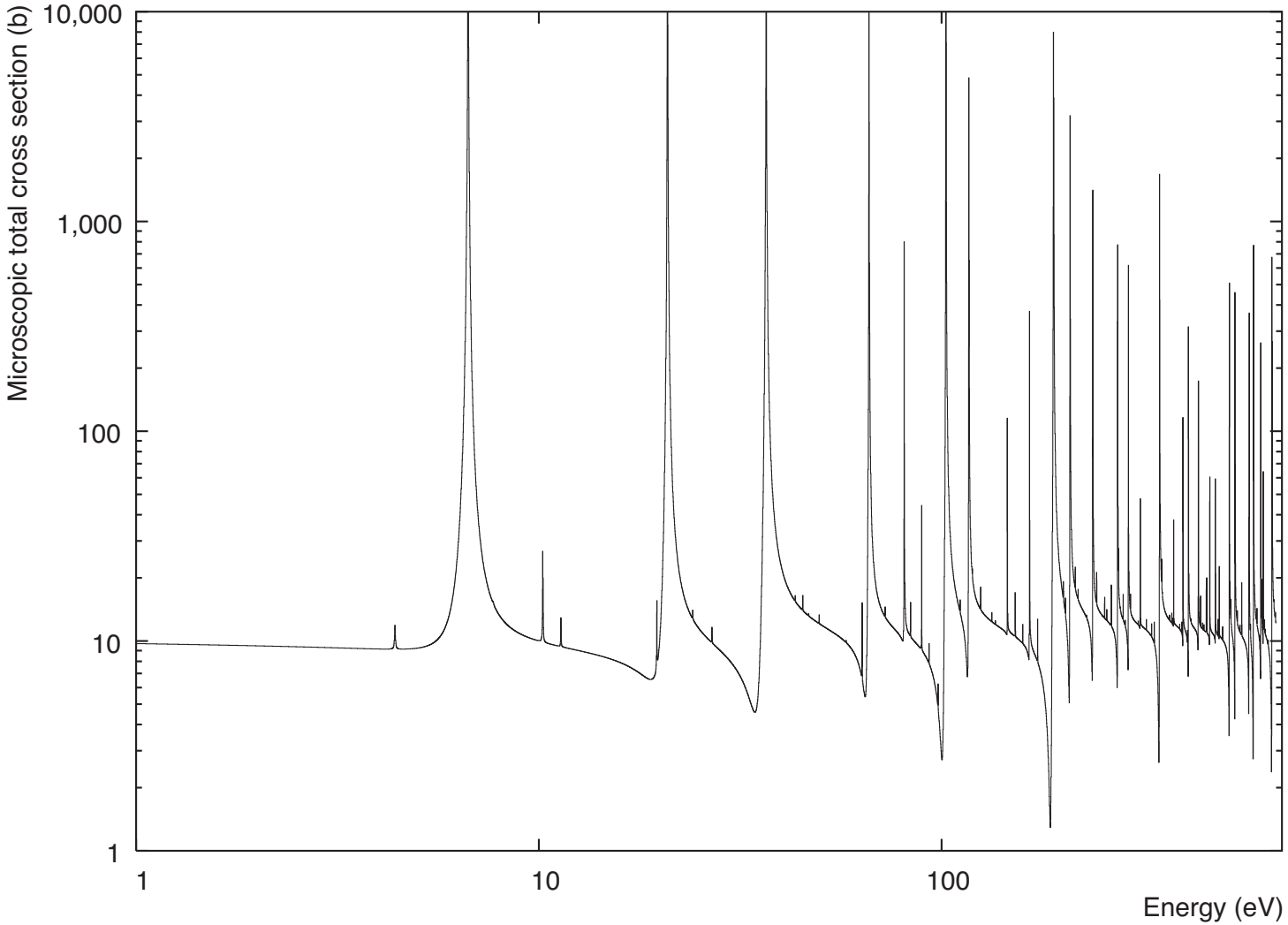
$$\delta\varphi(g,\sigma_e) = \varphi(g,\sigma_e) - 1 \quad (9)$$

where $I_{\mathrm{x}}(g,\sigma_e)$ is the effective resonance integral and $\varphi(g,\sigma_e)$ is the averaged fine structure function. Note that $\varphi(g,\infty) = 1$.

- `dragr` offers the possibility to include PENDF type information in the DRAGLIB file, to perform a more accurate self-shielding calculation in the resolved energy domain.
  - PENDF information is transformed into piecewise uniform cross sections defined over micro energy groups which form a super-set of the original group structure.
  - Each resonant isotope has a different micro-group structure.
  - This information is currently used with Riemann integration and CALENDF (mathematical probability tables) approaches.
  - This information is known as Autolib data.

The dragr module

Autolib data for U238



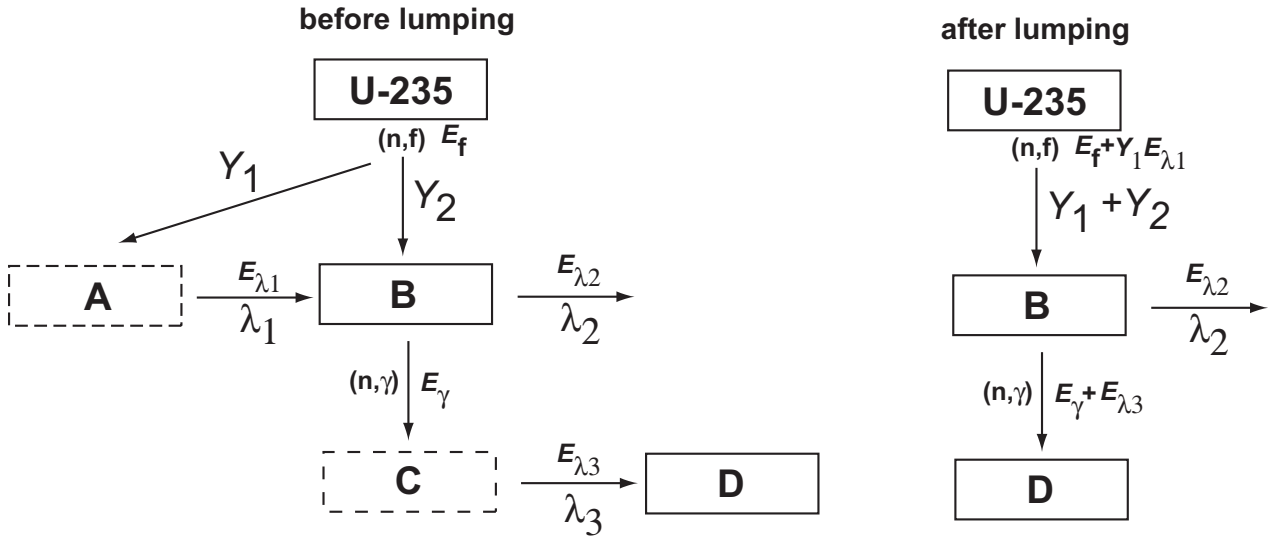
The dragr module

Burnup information

File 8 of ENDF evaluation contains half-lives, decay modes, decay energies, and radiation spectra for most isotopes. File 8 information is processed by module DRAGR.

- A large number of fission products are included in ENDF/B-VI rel. 8. One can notice that there are information of 1232 fission products for 0.0253 eV fission of ^{233}U, 1247 fission products for 0.0253 eV fission of ^{235}U etc.
- The evaluations are not available for all the nuclides, as most of them have very short half-lives and in the reactor context, can be considered insignificant.
- They are subsequently lumped by a procedure that is built in DRAGR and depicted in Figure.
- If there are nuclides with long half lives, but are not available as evaluated files, a warning is provided before lumping the corresponding element.
- The DRAGR user has the complete control over the lumping process.
- DRAGR currently has no capability to produce pseudo fission product.

The dragr module



- Energies for reaction types like (n, γ), (n, f), (n, xn), (n, $x\alpha$), (n, p), etc. are recovered from earlier DRAGR single-isotope calculations and included in relevant depletion data in DRAGLIB format.
- The fission energy (n, f) is obtained from MF1 MT458 and the energy from delayed betas and gammas are subtracted from it.
- Energies for other reactions are recovered from MF3.
- The complete information required to do the depletion calculations is provided in ten specific records of the DRAGLIB file.

Numerical results – dragr

- We have based our validation study on an eighth PWR assembly without leakage.
- All discrepancies presented in this section are evaluated with respect to the SERPENT2 code.
- Three types of fuel were studied, one UO_2 fuelled (UOX), one multi-zone $UPuO_2$ (MOX) and one UO_2 fuelled containing $UO_2Gd_2O_3$.
- Two SHEM-295 multigroup cross section libraries obtained using Njoy 99.364 and NJOY-2012.50, respectively.
- The table represents the effective multiplication factor for each type of fuel and for different computational options.
- Discrepancy between Njoy-99 and Njoy-2012 results is of the order of 1 pcm.

Table 1: k_{eff} and absolute discrepancies.

	UOX		MOX		$UO_2Gd_2O_3$	
	k_{eff}	Δa	k_{eff}	Δa	k_{eff}	Δa
SERPENT2	1.32392		1.12578		1.17368	
TRIPOLI4	1.32334	-58	1.12484	-94	1.17320	-48
DRAGON5/NJOY-99	1.32191	-201	1.12400	-178	1.17189	-179
DRAGON5/NJOY-2012	1.32190	-202	1.12399	-179	1.17188	-180

The WimsE framework

The WIMS-E library production framework is based on the PyNjoy 2012 system and on a simple utility named `willie5`, similar to the `willie` utility of the WLUP project. The PyNjoy 2012 system is made of the following components:

1. The NJOY-2012.0 distribution, as released by LANL.
2. Module `dragr` is not used for producing WIMS-formatted libraries.
3. New NJOY-2012 updates from École Polytechnique de Montréal (EPM). These updates contain
   - bug fixes
   - corrections for the `iverw=5` option of `wims` module.
   - additional energy meshes for the `groupr` module.
4. A generic Python script named PyNjoy.py for automating the preparation of datasets for NJOY. The script is used for
   - processing isotopes and
   - for constructing depletion chains.
5. A collection of Python datasets.
   - E. g.: `endfb7r0_shem281_wimsE.py`

The WimsE framework

The WIMS-D4 format shortcomings

The improvements obtained with a transition from WIMS-D4 to WIMS-E are:

- With the WIMS-D4 format, temperature-independent P_1 scattering cross sections are available only for four isotopes: H in H_2O, D in D_2O, ^{16}O and graphite. All other isotopes have transport-corrected P_0 scattering cross sections. With the WIMS-E format, all isotopes have both temperature-dependent P_0 and P_1 scattering cross sections.
- With the WIMS-D4 format, all fissile isotopes are using the same fission spectrum. With the WIMS-E format, each fissile isotope has a specific fission spectrum.
- (n,2n) cross sections are only available in a WIMS-E formatted library.
- Resonance tables for the scattering reaction are only available in a WIMS-E formatted library. With the WIMS-D4 format, cross sections other than absorption and fission are self-shielded at a fixed value given by the `sgref` parameter (selected during the NJOY run).

The WimsE framework

Resonances tables

Two-dimensional *resonance integral* tables are available in a WIMS-E library for three reactions: absorption, fission and scattering as a function of dilution σ_e and absolute temperature T. They are defined in energy group g as

$$\begin{aligned} I_{\mathrm{a},g}(\sigma_e,T) &= \bar{\sigma}_{\mathrm{a},g}(\sigma_e,T)\,\bar{\phi}_g(\sigma_e,T) \\ I_{\mathrm{f},g}(\sigma_e,T) &= \bar{\nu}\bar{\sigma}_{\mathrm{f},g}(\sigma_e,T)\,\bar{\phi}_g(\sigma_e,T) \\ I_{\mathrm{s},g}(\sigma_e,T) &= \bar{\sigma}_{\mathrm{s},g}(\sigma_e,T)\,\bar{\phi}_g(\sigma_e,T) \end{aligned} \tag{10}$$

respectively, where $\bar{\sigma}_{\rho,g}(\sigma_e,T)$ is the self-shielded cross section for reaction ρ, as computed by NJOY. The self-shielded flux in group g is defined as

$$\bar{\phi}_g(\sigma_e,T) = \frac{\sigma_e}{\sigma_e+\bar{\sigma}_{\mathrm{a},g}(\sigma_e,T)} = \frac{\sigma_e - I_{\mathrm{a},g}(\sigma_e,T)}{\sigma_e}. \tag{11}$$

Resonances tables for scattering $I_{\mathrm{s},g}(\sigma_e,T)$ are only available in a WIMS-E formatted library.

The WimsE framework

The self-shielded P_0 transfer cross sections are the product of the P_0 scattering law times the self-shielded scattering cross sections. They are assumed to be equal to

$$\bar{\sigma}_{\mathrm{s},h\leftarrow g}(\sigma_e, T) = \bar{\sigma}_{\mathrm{s},h\leftarrow g}(\infty, T)\,\frac{\bar{\sigma}_{\mathrm{s},g}(\sigma_e, T)}{\bar{\sigma}_{\mathrm{s},g}(\infty, T)} \tag{12}$$

where

$$\bar{\sigma}_{\mathrm{s},g}(\sigma_e, T) = \sum_h \bar{\sigma}_{\mathrm{s},h\leftarrow g}(\sigma_e, T). \tag{13}$$

- Equation (12) is an approximation related to the choice of the WIMS-E library format.
- Approximation (12) is avoided in `dragr` and in DRAGLIB libraries.
- Approximation (12) is avoided in `matxsr` and in MATXS libraries (Los Alamos format).
- Approximation (12) is used in cross-section libraries for the APOLLO2 code.

The WimsE framework

wimsr module update

The following update is proposed in NJOY version 2012.82 to support `iverw` = 5 in `wimsr` module:

```
*/ wimsr -- 2october2016
*/ correct bugs related to iverw=5 implementation
*d wimsr.34
   integer::ifiss,ifissr,nfiss
*d wimsr.438
   real(kr)::xid,siglam,sigb,siga,sigs,sig
*i wimsr.450
   ifissr=0
*i wimsr.522
   if ((mth.gt.50).and.(mth.le.91)) go to 162
*d wimsr.541
*d wimsr.582,wimsr.583
   !--elastic or inelastic scattering
   else if ((mth.eq.2).or.((mth.gt.50).and.(mth.le.91))) then
*i wimsr.588
   else
      go to 300
*i wimsr.664
            sigs=elas(loc+iz-1)
*i wimsr.666
            if (iverw.ne.4) elas(loc+iz-1)=sigb*sigs/(sigb+siga)
*i wimsr.671
   ifissr=jfiss
*i wimsr.932
   if (iverw.eq.5) isg=1
*i wimsr.2043
   if((ifis.eq.3).and.(ifissr.ne.3)) ifis=2
```

PyNjoy tutorial – wimsr

En example of PyNjoy dataset for processing ^{238}U from ENDF/B-VIIr0 with a SHEM281energy mesh follows (`wimsr`–specific data is in blue):

```
#!/usr/local/bin/python
from PyNjoy import *
from os import uname
endfb = PyNjoy()
endfb.evaluationName = "/tmp/shem281_endfb7r0_u238wimsE"
endfb.execDir = "../" + uname()[0]
endfb.nstr = 24
endfb.iwt = -4
endfb.autolib = (22.53556, 1345.061, 0.001)
endfb.jp1 = 0
endfb.iverw = 5
endfb.yields = None
endfb.purr = None
endfb.scatteringLaw = None
endfb.temperatures = ( 293., 550., 900., 1200., 2000. )
endfb.eFiss = None
endfb.legendre = 0

endfb.hmat = "U238"
endfb.mat = 9237
endfb.evaluationFile = "$HOME/evaluations/ENDFB7r0/n-ENDF-VII0.endf/n-092_U_238.endf"
endfb.fission = 2 # fission with delayed neutrons
endfb.potential = 11.8237
endfb.dilutions = ( 1.e10, 2.e4, 3.6e3, 1.0e3, 2.6e2, 140., 64., 52., 28., 10.)
endfb.pendf()
endfb.gendf()
endfb.wmat = 92238
endfb.goldstein = 0.2
endfb.wims()
```

PyNjoy tutorial – wimsr

The output of Njoy-2012 execution is

```
Alains-MacBook-Pro:python alainhebert$ python endfb7r0_shem281_u238wimsE.py
 --- make pendf for U238 ---
 njoy 2012.82  20jan17                                          04/13/17 10:11:12
 ************************************************************************
 moder...                                                              0.0s

 reconr...                                                             0.1s

 broadr...                                                           183.1s
      293.0 deg                                                      183.9s
      550.0 deg                                                      203.1s
      900.0 deg                                                      225.2s
     1200.0 deg                                                      250.2s
     2000.0 deg                                                      277.4s

 unresr...                                                           309.1s

 thermr...                                                           310.3s
 wrote thermal data for temp = 2.9300E+02                            313.8s
 wrote thermal data for temp = 5.5000E+02                            317.2s
 wrote thermal data for temp = 9.0000E+02                            320.5s
 wrote thermal data for temp = 1.2000E+03                            323.7s
 wrote thermal data for temp = 2.0000E+03                            326.9s

 moder...                                                            326.9s
                                                                     397.5s
 ************************************************************************
```

PyNjoy tutorial – wimsr


```
--- make gendf for U238 ---
njoy 2012.82  20jan17                                        04/13/17 10:17:55
******************************************************************************
moder...                                                                 0.0s

moder...                                                                 0.0s

groupr...                                                                6.8s

moder...                                                               148.4s
                                                                       149.7s
******************************************************************************
--- make wimslib for U238 ---
njoy 2012.82  20jan17                                        04/13/17 10:20:27
******************************************************************************
moder...                                                                 0.0s

wimsr...                                                                 0.2s
---message from wminit---mat 9237 mf  3 has both mt18 and mt19
                          mt18 will be used
---message from wminit---mat 9237 has no mf3, mt252
                          isotropic c.m.scattering will be assumed
                                                                         0.3s
******************************************************************************
```

Scattering resonance information

- Scattering resonance information in the Wimslib is generally computed at infinite dilution.
- It is possible to select a dilution smaller than infinity by setting the `sgref` variable in `wimsr` module to a value chosen in the set of dilutions used by the `groupr`, `unresr` or `purr` modules.
- The WLUP libraries in WIMS-D4 format use `sgref` = 28 barn for U238 and `sgref` = 800 barn for U235. The PyNjoy data for U238 used by the WLUP project is

```
endfb.iverw = 4
endfb.sgref = 28.0
```

- A study made with DRAGON5 leads to the following dilution values for U238:

Case	U238 average dilution (barn)
Rowlands UOX pincell	65.0
Rowlands MOX pincell	77.0
UOX 17×17 PWR assembly	135.0
MOX 17×17 PWR assembly	135.0

The willie5 utility

- The NJOY output is a set of ASCII files, one per isotope, located in directory `/tmp/shem281_endfb7r0_u238wimsE/`.
- The following operations remains to be done:
  - Concatenate all the isotopic directories
  - Construct the depletion data for the library
  - Convert the library to binary WIMS-E format

The `willie5` utility is a simple conversion tool for a WIMSLIB in WIMS-E format. It has three commands:

`MAKE`: Catenate the individual isotopic WIMSLIB outputs from the `wimsr` module of NJOY (executed with `iverw` = 5) into a single ASCII library in WIMS-E format

`FOBI`: Convert a WIMS-E library from ASCII to sequential binary format.

`END`: End the processing

The willie5 utility

The Willie5 utility executes in a console (user's commands are in blue):

```
Alains-MacBook-Pro:willie5 alainhebert$ ./willie5
$Enter wimslib version (4 or 5)
5
$Enter the selected option
MAKE
$Process option MAKE
$Enter NJOY working directory:
/tmp/shem281_endfb7r0_u238wimsE/
$Enter input Wimslib-E ascii name [wimslib_out.txt]:
libshem281_endfb7r0_u238wimsE.txt
$number of nuclides in NJOY working directory=    1
$Process isotopic wimslib:  /tmp/shem281_endfb7r0_u238wimsE/wimslibU238
$Number of fission products=    0
$Number of fissile isotopes=    0
$End of NJOY directory processing: /tmp/shem281_endfb7r0_u238wimsE/
$Enter the selected option
FOBI
$Process option FOBI
$Enter input Wimslib-E ascii name [wimslib_out.txt]:
libshem281_endfb7r0_u238wimsE.txt
$Enter output Wimslib-E binary name [wimslib_out.bin]:
libshem281_endfb7r0_u238wimsE.bin
$Process isotope  92238
$Enter the selected option
END
$Successful end of processing
```

Rowlands benchmark results

We have based our validation study on a subset made up of eight Rowlands pin-cell benchmark cases.

- The comparisons were made for light-water reactor pin-cells without leakage.
- Two types of pin-cell were studied,
  - UO_2 fuelled (UOX),
  - $UPuO_2$ fuelled, in two versions with different isotopic compositions (MOX–1 and MOX–2).

UOX case 1: Isothermal 293 K
UOX case 2: Reduced H2O Density
UOX case 3: Fuel at 900 K
UOX case 4: Isothermal 574 K
MOX case 1: MOX Fuel 1,Isothermal 300 K
MOX case 2: MOX Fuel 1, Fuel at 560 K
MOX case 3: MOX Fuel 2,Isothermal 300 K
MOX case 4: MOX Fuel 2, Fuel at 560 K

Rowlands benchmark results

K_{eff} results

	UOX case 1	UOX case 2	UOX case 3	UOX case 4
WIMS-D4				
`sgref` = 28 b	1.385201	1.330805	1.295787	1.309841
`sgref` = 64 b	1.385240	1.330844	1.295833	1.309883
`sgref` = 140 b	1.385305	1.330916	1.295913	1.309958
`sgref` = 20000 b	1.386631	1.332373	1.297506	1.311475
`sgref` = 1.0×10^{10} b	1.386865	1.332636	1.297788	1.311745
WIMS-E	1.385100	1.330629	1.295625	1.309671
DRAGLIB	1.385281	1.330901	1.295877	1.309990

	MOX case 1	MOX case 2	MOX case 3	MOX case 4
WIMS-D4				
`sgref` = 28 b	1.223384	1.207996	1.268746	1.254351
`sgref` = 64 b	1.223392	1.208006	1.268759	1.254367
`sgref` = 140 b	1.223406	1.208025	1.268781	1.254400
`sgref` = 20000 b	1.223767	1.208515	1.269336	1.255093
`sgref` = 1.0×10^{10} b	1.223824	1.208600	1.269433	1.255219
WIMS-E	1.223208	1.207827	1.268565	1.254176
DRAGLIB	1.223446	1.208057	1.268818	1.254421

Rowlands benchmark results

- In the case of pin-cell UOX Rowlands benchmark, the average dilution of ^{238}U isotope can be estimated around 100 barn. The expected result should therefore correspond to the WIMS-D4 calculation with `sgref` = 140 b.
- The corresponding K_{eff} is consistent with the value obtained with a DRAGLIB, but is 20 to 30 pcm above the WIMS-E result.
- This discrepancy with the WIMS-E library is due to the approximation in Eq. (3) which consists to neglect the self-shielding of the scattering law (but *not* to neglect the self-shielding of the scattering cross section).
- Similar conclusions can be made about the MOX results.

Conclusions for WIMS-E support

- We are proposing a framework to upgrade from WIMS-D4 to WIMS-E library format.
- Such a replacement would improve the overall quality of the cross section data used in lattice codes actually based on WIMS-D4 libraries.
- The similarity between the two formats would facilitate the software modifications inside the lattice codes (few weeks work to make the modifications).
- Capability to read WIMS-E formatted libraries is available in DRAGON version 5.0.3 and up.
- The complete system (with the exception of the initial NJOY-2012.0 source) is and will remain openly available and developed under the Lesser General Public License and is available on site `http://merlin.polymtl.ca/`.
- The current implementation is based on update 82 of NJOY-2012.

Ressources

PyNjoy2012 distribution:

`https://merlin.polymtl.ca/pynjoy2012.htm`

Draglib libraries:

Use `DRAGON` keyword in module `LIB:` of DRAGON5.

`https://merlin.polymtl.ca/libraries.htm`

WIMSE libraries:

Use `WIMSE` keyword in module `LIB:` of DRAGON5.

- SHEM-281, ENDF/B-VII r0, little endian (gz)
- SHEM-281, ENDF/B-VII r0, big endian (gz)
- Willie5 system for processing WIMSE libraries (tgz)

Ressources

PyNjoy 2012 is available on page `http://merlin.polymtl.ca/pynjoy2012.htm`

About PyNjoy 2012

POLYTECHNIQUE MONTRÉAL

$Updated: 2015/12/29$

The PyNjoy 2012 system

The PyNjoy 2012 system is a set of components dedicated to the production of cross-section libraries in Draglib format for the DRAGON lattice code. These libraries can be used with Version3, Version4 and Version5 distributions. The PyNjoy 2012 system produces a Draglib in ASCII format that can be converted in binary XSM format by the equality module (`:=`) available in DRAGON. PyNjoy 2012 also offers limited support for producing libraries in Wimslib or Acelib format. The PyNjoy 2012 is based on Njoy 2012.

Important note: You need a valid Njoy 2012 license from Los Alamos National Laboratory (LANL) in order to use the PyNjoy 2012 system.

The PyNjoy 2012 system is made of the following components:

1. The Njoy 2012.0 distribution, as released by LANL[1]. Note that the source of Njoy 2012.0 has been removed from the PyNjoy archive. If you want to use the library production system, you have to rename the Njoy 2012.0 source (`src` file) as `src_2012p0` and to move it in directory `Njoy2012_EPM/`. Next, follow the instructions in the `Njoy2012_EPM/readme` file.
2. A new module named `dragr` in PyNjoy 2012 for producing Draglib files from endf, pendf and gendf information. The `dragr` module is presented in Sect. 2.9.2 of Ref. [2].
3. New Njoy 2012 updates from École Polytechnique de Montréal. These updates contain bug fixes and additional energy meshes for the `groupr` module:
   i. **SHEM-281:** Santamarina-Hfaiedh 281-group energy mesh used at the Commissariat à l'Énergie Atomique (CEA), Areva, and Électricite de France (EDF)[3].
   ii. **SHEM-361:** 361-group energy mesh defined as a collaboration between the CEA and École Polytechnique de Montréal (EPM)[4].
   iii. **SHEM-295:** 295-group energy mesh defined at EPM.
   iv. **SHEM-315:** 315-group energy mesh defined at EPM.
   v. **Rahab-89:** 89-group energy mesh defined at Atomic Energy of Canada Limited (AECL).
4. A generic Python script named `PyNjoy.py` for automating the preparation of datasets for Njoy. Processing of complete ENDF evaluations is greatly facilitated with the help of this script. The script is used for processing isotopes and for constructing depletion chains.
5. A collection of Python datasets, each of them corresponding to a specific evaluation (Jef2.2, Jeff3.1, ENDFB-VII rel. 0, etc.) processed with a specific multigroup energy mesh (XMAS-172, SHEM-281, etc.).

Download PyNjoy 2012 components

The available components in the PyNjoy 2012 distribution are:

- Njoy 2012 user's guide with modifications (PDF)
- PyNjoy tutorial (PDF)
- PyNjoy 2012 archive. To expand the archive, type "`tar xvfz arch_njoy2012_epm_up50.tgz`".

modified up50 archive	tgz	2015/12/29
modified up82 archive	tgz	2017/04/12
modified up99 archive	tgz	2017/08/22
modified up137 archive	tgz	2018/10/10

- Open-source Draglibs in XMAS or SHEM binary formats. If you want to download such a multigroup cross-section library in Draglib format, please go here.