M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017, on USB (2017)

A Proposal Beyond the Wims Library Update Project

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Abstract - *We are proposing a new open-source framework for producing WIMS-E formatted libraries based on the NJOY-2012 package from LANL. Currently, many general-purpose cross section libraries are produced in the WIMD-D4 format, using tools available in the Wims Library Update Project (WLUP). However, this library format suffers from many limitations that were mostly corrected with the WIMS-E library format. We are presenting the limitations of the WIMS-D format and the improvements obtained with the WIMS-E format. Our new open-source framework has capabilities similar to those of the WLUP project, but is dedicated to the WIMS-E format.*

I. INTRODUCTION

The objective of the WIMS-D Library Update Project (WLUP) was to provide updated working libraries compatible with the WIMS-D family of codes or equivalent lattice cell codes.[1] This would enable scientists and reactor designers to make use of the most recent evaluated nuclear data files for research and power thermal reactor calculations. The WLUP project was allocating a large amount of resources over years to provide open-source software tools, documentation and cross-section libraries that are currently used in lattice codes such as WIMS-D4 and DRAGON.[2, 3] More recently, the WLUP framework was used to develop an industrial cross section library for the Chinese LATC lattice code of COSINE software package.[4]

All these valuable contributions rely on the WIMS-D library format, consistent with a processing of the ENDF/B evaluation by the `wimsr` module of NJOY with flag `iverw` set to 4.[5] However, this library format suffers from many limitations that were mostly corrected with the WIMS-E library format. We are presenting the limitations of the WIMS-D format and the improvements obtained with the WIMS-E format.

The WIMD-E format library was previously used and possibly improved by the WIMS-7 project, back in 1996.[6] This project is still alive under control by ANSWERS Software Service of Amec Foster Wheeler in UK.[7] Today, the WIMS Datagram Utility routines process the evaluated nuclear data produced by NJOY into the datagram format specifically for use with the latest version of WIMS. This processing route is an internal capability within ANSWERS. Amec Foster Wheeler do not allow users to generate their own WIMS nuclear data libraries. Any information related to WIMS10 is subject to strict UK export licence, commercial and NDA controls.

École Polytechnique de Montréal is proposing an alternative framework for producing WIMS-E libraries under an open-source license. This framework for generating WIMS-E formatted cross-section libraries is based on NJOY and on a new WLUP-type utility named `willie5`. These tools are presented and numerical tests based on the Rowlands benchmark are used to illustrate the main improvement gained with the new format. A comparison is proposed between DRAGON5 runs based on WIMS-D4, WIMS-E and DRAGLIB (see Sect. 2.9.3 of Ref. [8]) formatted libraries.

II. THE WIMS-E LIBRARY PRODUCTION FRAMEWORK

The WIMS-E library production framework is based on the PyNjoy 2012 system[9] and on a simple utility named `willie5`, similar to the `willie` utility of the WLUP project.[1] 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. The `dragr` module is presented in Sect. 2.9.2 of Ref. [8]. The flowchart of NJOY-2012 processing, including `dragr`, is presented in Fig. 1.
3. New NJOY-2012 updates from École Polytechnique de Montréal (EPM). These updates contain bug fixes and additional energy meshes for the `groupr` module. Among these, the SHEM-281 mesh is the Santamarina-Hfaiedh 281-group energy mesh used at the Commissariat à l'Énergie Atomique (CEA), Areva, and Électricite de France (EDF).[10].
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.).

We found that corrections have to be made to the `wimsr` module of NJOY version 2012.50 in order to correctly process cross sections with flag `iverw` set to 5. The following update is proposed:

```
*/ 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
```

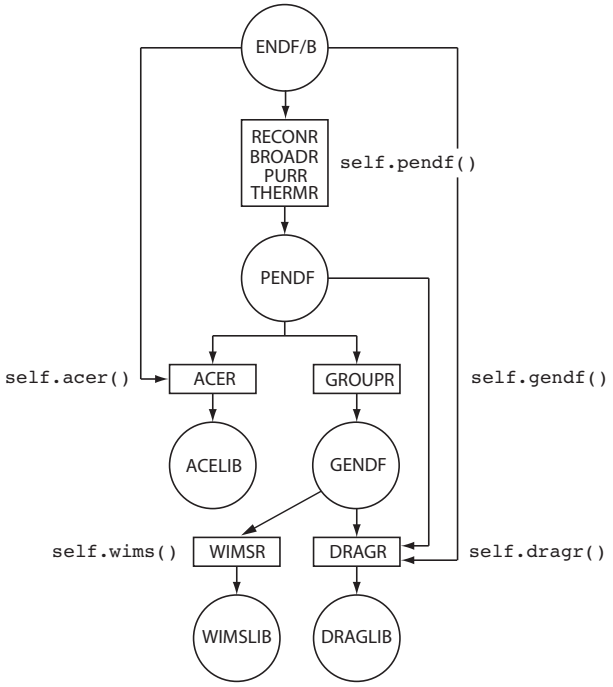

Fig. 1. Dataflow of cross-section library processing with NJOY-2012.

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

III. UPGRADING FROM WIMD-D4 TO WIMS-E LIBRARY FORMAT

The WIMS-D4 library specification format suffers from many drawbacks that were mostly corrected in the WIMS-E specification. Both WIMS-D4 and WIMS-E formats share a similar layout of cross-section data and nearly identical depletion information. Any lattice code based on WIMS-D4 cross sections can be easily modified to the new format. Capability to process WIMS-E formatted cross sections was implemented in version 5.0.3 of the DRAGON5 lattice code. 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).

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

$$\begin{aligned} I_{\mathrm{a},g}(\sigma_e,T) &= \bar{\sigma}_{\mathrm{a},g}(\sigma_e,T)\,\bar{\phi}_g(\sigma_e,T) \\ I_{\mathrm{f},g}(\sigma_e,T) &= \nu\bar{\sigma}_{\mathrm{f},g}(\sigma_e,T)\,\bar{\phi}_g(\sigma_e,T) \\ I_{\mathrm{s},g}(\sigma_e,T) &= \bar{\sigma}_{\mathrm{s},g}(\sigma_e,T)\,\bar{\phi}_g(\sigma_e,T) \end{aligned} \quad (1)$$

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

$$\bar{\phi}_g(\sigma_e,T) = \frac{\sigma_e}{\sigma_e + \bar{\sigma}_{\mathrm{a},g}(\sigma_e,T)} = \frac{\sigma_e - I_{\mathrm{a},g}(\sigma_e,T)}{\sigma_e}. \quad (2)$$

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

$$\bar{\sigma}_{\mathrm{s},h\leftarrow g}(\sigma_e,T) = \bar{\sigma}_{\mathrm{s},h\leftarrow g}(\infty,T)\,\frac{\bar{\sigma}_{\mathrm{s},g}(\sigma_e,T)}{\bar{\sigma}_{\mathrm{s},g}(\infty,T)} \quad (3)$$

where

$$\bar{\sigma}_{\mathrm{s},g}(\sigma_e,T) = \sum_h \bar{\sigma}_{\mathrm{s},h\leftarrow g}(\sigma_e,T). \quad (4)$$

Equation (3) is an approximation related to the choice of the WIMS-E library format. The same approximation is also used with other library format, such as the APOLIB-2 format. Using a more complete library format based on the DRAGLIB specification, it is possible to store resonance tables for each component of the transfer cross-section matrix and to avoid this approximation.

IV. NUMERICAL RESULTS

We have based our validation study on a subset made up of eight Rowlands pin-cell benchmark cases.[11] The comparisons were made for light-water reactor pin-cells without leakage. Two types of pin-cell were studied, one UO_2 fuelled (UOX), and the other $UPuO_2$ fuelled, the latter in two versions with different isotopic compositions (MOX–1 and MOX–2). The temperature of water was slightly modified to correspond to the $S(\alpha,\beta)$ tabulation points of the ENDF/B-VII evaluation.

	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

TABLE I. DRAGON5 K_{eff} results obtained on the Rowlands UOX benchmarks.

The UOX and MOX calculations use the same multigroup cross-section library based on the ENDF/B-VII r0 evaluation processed with a SHEM-281 multigroup energy mesh definition.[10] A WIMS-E formatted cross section library for all isotopes present in the benchmark was produced from scratch with NJOY[5] release 2012.50. The ^{238}U isotope was also processed alone in WIMS-D4, WIMS-E and DRAGLIB formats using the same PENDF file as input. Many instances of the WIMS-D4 library for ^{238}U were created for different values of the `sgref` parameter, selected in set (28 b, 64 b, 140 b, 20000 b and 1.0×10^{10} b). In this case, the correct fission spectrum is used for ^{238}U, avoiding a 12 to 20 pcm error if a ^{235}U spectrum is used for ^{238}U. The Goldstein-Cohen parameter of ^{238}U is set to 0.2 in the DRAGON5 dataset in cases where a DRAGLIB library is used. All DRAGON5 pin-cell calculations are solved using the collision probability method and all resonant isotopes are self-shielded using the generalized Stamm'ler method without Livolant-Jeanpierre normalization and without taking into account distributed self-shielding effects.[12] These simplifications in the self-shielding model may introduce inaccuracies in the reported K_{eff} results, without compromising the consistency of the library comparisons.

Numerical results for the UOX benchmarks are presented

in Table I. 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). This approximation is avoided if a DRAGLIB is used or if a WIMS-D4 library is constructed at a specific `sgref` value.

	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

TABLE II. DRAGON5 K_{eff} results obtained on the Rowlands MOX benchmarks.

Numerical results for the MOX benchmarks are presented in Table II. Similar conclusions can be made about the effect of neglecting self-shielding of the scattering law with a WIMS-E library. In this case, the underestimation of the K_{eff} is of the order of 25 pcm.

V. CONCLUSION

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. 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://www.polymtl.ca/merlin/`.

REFERENCES

1. F. LESZCZYNSKI, D. LÓPEZ ALDAMA and A. TRKOV, "WIMS-D Library Update," International Atomic Energy Agency Report STI/PUB/1264, Vienna, Austria (2007).
2. J. R. ASKEW, F. J. FAYERS and P. B. KEMSHELL, "A General Description of the Lattice Code WIMS," *J. British Energy Society*, **5**, 564 (1966).
3. A. HÉBERT, "DRAGON5 and DONJON5, the contribution of École Polytechnique de Montréal to the SALOME platform," *Ann. nucl. Energy*, **87**, 12–20 (2016). See the home page at `http://www.polymtl.ca/merlin/`.
4. Y. YAN, "Application and research of 281 group cross section library to lattice physics code of COSINE software package," *Int. Conf. On Nuclear Data for Science and Technology (ND2016)*, Bruges, Belgium, September 11–16, 2016.
5. R. E. MACFARLANE and A. C. KAHLER, "Methods for Processing ENDF/B-VII with NJOY," *Nuclear Data Sheets*, **111**, 2739 (2010).
6. M. J. HALSALL, "WIMS7, An Overview," *Proc. Int. Conf. on the Physics of Reactors—PHYSOR 96*, Mito, Japan, p. B-1, September 16–20 (1996).
7. B. A. LINDLEY, T. D. NEWTON, J. G. HOSKING, P. N. SMITH, D. J. POWNEY, B. TOLLIT and P. J. SMITH, "Release of WIMS10: A Versatile Reactor Physics Code for Thermal and Fast Systems," Proceedings of ICAPP 2015, Nice, France, May 3–6, 2015.
8. A. HÉBERT, *Applied Reactor Physics*, second edition, Presses Internationales Polytechnique, ISBN 978-2-553-01698-1, 396 p., Montréal, 2016. See the home page at `http://www.polymtl.ca/pub/`.
9. A. HÉBERT, "PyNjoy 2012 : A system for producing cross-section libraries for the DRAGON lattice code," *Int. Conf. On Nuclear Data for Science and Technology (ND2016)*, Bruges, Belgium, September 11–16, 2016.
10. N. HFAIEDH and A. SANTAMARINA, "Determination of the Optimized SHEM Mesh for Neutron Transport Calculations," *Proc. Topical Meeting in Mathematics & Computations, Supercomputing, Reactor Physics and Nuclear and Biological Applications*, September 12 – 15, Avignon, France, 2005.
11. J. ROWLANDS et al, "LWR Pin Cell Benchmark Intercomparisons. An Intercomparison study organized by the JEF Project, with contributions by Britain, France, Germany, The Netherlands, Slovenia and the USA.," *JEF Report to be published* , OECD/NEA Data Bank (1999).
12. A. HÉBERT and G. MARLEAU, "Generalization of the Stamm'ler Method for the Self-Shielding of Resonant Isotopes in Arbitrary Geometries," *Nucl. Sci. Eng.*, **108**, 230 (1991).