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AN ALTERNATIVE APPROACH TO CREATING ACE DATA FILES FOR USE IN MONTE CARLO CODES

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Introduction

There is a strong desire in Member States to have access to "open source" data processing system that would be well maintained and would avoid the danger of "common mode failure" due to all data processing done with the same set of processing tool. At present, the only tool for generating libraries in ACE format for Monte Carlo transport codes is the NJOY data processing system [1]. Self-shielding in the unresolved resonance range (URR) is treated by the probability table method (PTM) [7, 8, 9], generated from statistically distributed ladders of resonances. If other codes could generate equivalent parameters, this would open the door to an alternative route for generating the ACE libraries.

The methodology in PREPRO codes [2] can produce multi-band parameters (MB) from self-shielded cross sections [5, 6]. The multi-band parameters have been used in the TART Monte Carlo code [3] and in deterministic codes [4], for many years, but they were not applied broadly in other codes. The multi-band parameters were shown to be equivalent to the probability tables like those generated by the PURR module of NJOY. Generally two bands are here shown to be sufficient, in contrast to the probability tables in PURR, which typically use about 20 bins to represent the probabilities.

The purpose of the present work is to show that the replacement of the probability tables in ACE files with two band parameters (based on the same self-shielded cross sections) reproduces reference results for the criticality of reactor assemblies with sufficient precision.

Positive results of the exercise justify the development of alternative modules for generating multi-band parameters in the unresolved resonance range, and possibly extending the multi-band approach to lower energies in order to reduce the volume of the ACE libraries without sacrificing the accuracy of the calculations.

Method

The self-shielded cross sections generated by the PURR module of NJOY (denoted by MF2/MT152 in the intermediate PENDF file) are used to generate two-band parameters to replace the probability tables of PURR (denoted by MF2/MT153). The modified file is then used to assemble the full ACE library with the ACER module of NJOY. The nuclides ^{235}U and ^{238}U were taken as an example. Three ACE files were generated for each nuclide:

- Straightforward processing with NJOY to make the reference case.
- Same as above, but substituting parameters that produce “no self-shielding” in the URR.
- Processing with NJOY, but substituting the PTM parameters in the PENDF file produced by the PURR module with the two-band parameters that reproduce the self-shielded cross sections generated by PURR, using the URRDO code (available on request from D.E. Cullen).

Test cases

The test cases included in the analysis were selected from the ICSBEP Handbook according to the following criteria:

- Benchmarks that are sensitive to the capture and fission of the two uranium isotopes in the epithermal energy region; the search for such benchmarks was done with the DICE package, that is available with ICSBEP (version 2014).
- Benchmarks that are sensitive to capture in ^{238}U in the energy region from 10 keV to 20 keV (the list was provided by O. Cabellos, OECD/NEA Data Bank).
- Availability of inputs for MCNP.
- Godiva benchmark was added because it is the most widely used benchmark.

The complete list of benchmarks is given in Table 1.

Table 1: List of benchmarks included in the analysis.

No.	ICSBEP label	Short name	Common name
1	HEU-MET-FAST-001	hmf001	Godiva
2	HEU-MET-FAST-002	hmf002-2	Topsy-2
3	HEU-MET-FAST-003	hmf003-01	Topsy-U_2.0in(Uranium reflector)
4	HEU-MET-FAST-003	hmf003-02	Topsy-U_3.0in(Uranium reflector)
5	HEU-MET-FAST-003	hmf003-03	Topsy-U_4.0in(Uranium reflector)
6	HEU-MET-FAST-003	hmf003-10	Topsy-W_4.5in(Tungsten reflector)
7	HEU-MET-FAST-003	hmf003-11	Topsy-W_6.5in(Tungsten reflector)
8	HEU-MET-FAST-014	hmf014	VNIIEF-CTF-DU
9	HEU-MET-FAST-032	hmf032-1	COMET-TU1_3.93in
10	HEU-MET-FAST-032	hmf032-2	COMET-TU1_3.52in
11	HEU-MET-FAST-032	hmf032-3	COMET-TU1_1.742in
12	HEU-MET-FAST-032	hmf032-4	COMET-TU1-0.683in
13	IEU-MET-FAST-007	imf007	Big_Ten
14	IEU-MET-FAST-007	imf007d	Big_Ten(detailed)
15	IEU-MET-FAST-010	imf010	ZPR-6/9(U9)
16	IEU-MET-FAST-013	imf013	ZPR-9/1(Tungsten reflector)
17	IEU-MET-FAST-014	imf014-2	ZPR-9/2(Tungsten reflector)
18	MIX-MISC-FAST-001	mif001-01	BFS-35-1
19	MIX-MISC-FAST-001	mif001-02	BFS-35-2
20	MIX-MISC-FAST-001	mif001-03	BFS-35-3
21	MIX-MISC-FAST-001	mif001-09	BFS-31-4
22	MIX-MISC-FAST-001	mif001-10	BFS-31-5
23	MIX-MISC-FAST-001	mif001-11	BFS-42
24	IEU-MET-FAST-022	imf022-01	FR0_3X-S
25	IEU-MET-FAST-022	imf022-02	FR0_5-S
26	IEU-MET-FAST-022	imf022-03	FR0_6A-S
27	IEU-MET-FAST-022	imf022-04	FR0_7-S
28	IEU-MET-FAST-022	imf022-05	FR0_8-S
29	IEU-MET-FAST-022	imf022-06	FR0_9-S
30	IEU-MET-FAST-022	imf022-07	FR0_10-S
31	IEU-MET-FAST-012	imf012	ZPR-3/41
32	IEU-COMP-FAST-004	icf004	ZPR-3/12

Results

All calculations with MCNP were done with identical inputs. The number of source particles was sufficient to reach uncertainties below 8 pcm (parts per 100 000). A few selected cases were re-run with an increased number of particles to pin-down statistically significant differences. The results can be summarized as follows:

- Fast bare systems are insensitive to the self-shielding in ^{235}U and ^{238}U in the URR range.
- Fast systems reflected by natural or depleted ^{238}U show some sensitivity, but generally the impact of URR self-shielding amounts to less than 100 pcm.
- The most sensitive are intermediate-enriched uranium systems, where in some cases the impact exceeds 1000 pcm (e.g. the BSF_35-1, BSF_31-2 and BSF_31-3 benchmarks). The well-known Big_Ten assembly shows a sensitivity of about 400 pcm (see Figure 1).
- In most of the cases the calculations with probability tables and with two-band parameters were statistically indistinguishable, with differences that were generally well below 20 pcm and well within two-sigma uncertainty. Potential real differences were suspected in two cases with significant sensitivity to self-shielding of about 500 pcm, namely BSF_31-4 and BSF_31-5. The runs for these assemblies were repeated to reach a statistical uncertainty of 3 pcm in each run. The difference between the calculations with probability tables and with two-band parameters were 18 pcm and 15 pcm, respectively, with a combined uncertainty of 6 pcm each.

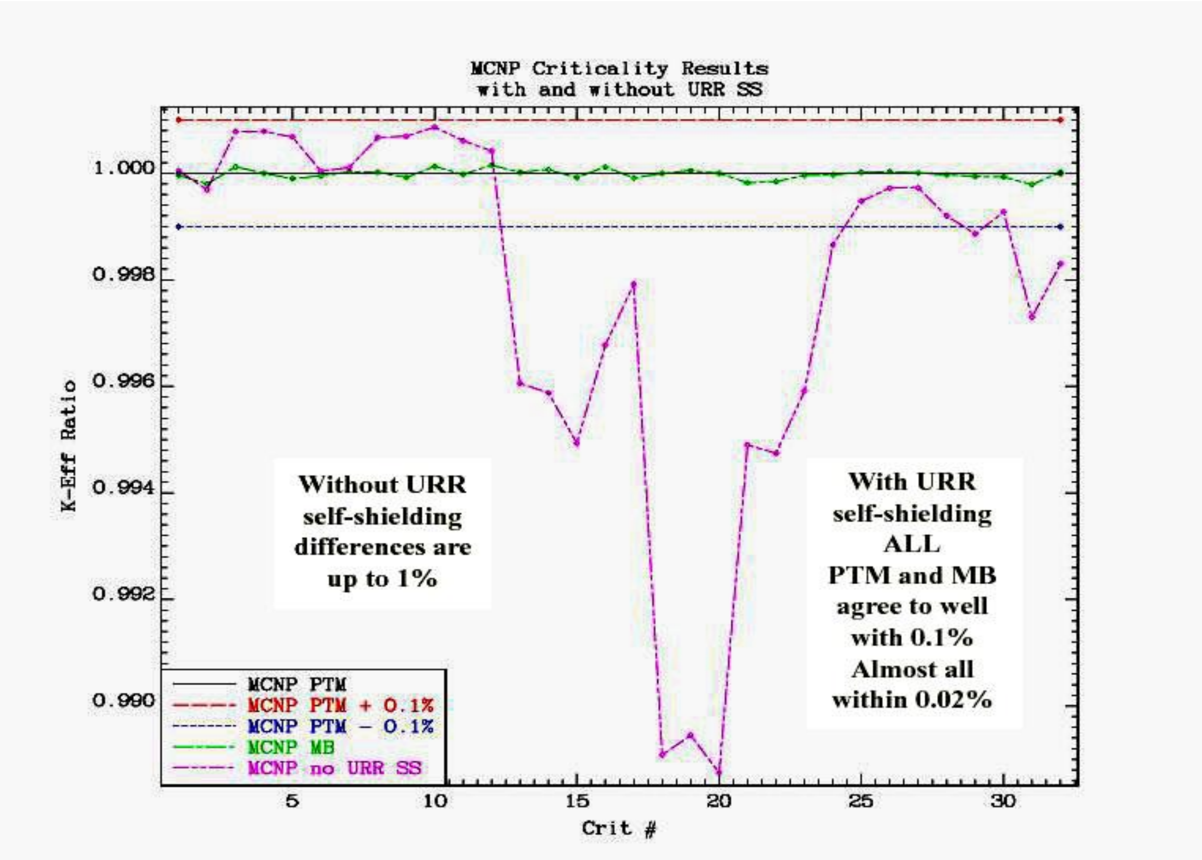

***Fig. 1**: Calculated k_{eff} ratios to the reference calculation with PTM parameters of the calculation without self-shielding (purple) and with PTM parameters replaced by two-band MB parameters (green).*

Conclusion

The overall conclusion is that two-band parameters can be substituted for the probability tables in the ACE libraries for Monte Carlo transport calculations. Out of the 32 benchmark criticality cases sensitive to epithermal capture and fission in ^{235}U and ^{238}U the maximum difference in the results was about 20 pcm, which is much smaller in comparison to the actual uncertainties in real systems.

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