Multipole-based Cross-section Library for Monte Carlo Code MCS

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1. Introduction

For high fidelity simulations of recent nuclear systems, coupling calculations of neutron transport, thermal hydraulics, fuel performance, and nuclear chemistry codes are needed to achieve the detail predictions of nuclear reactor cores. One important issue is to consider the temperature feedback corresponding to different temperature distribution of each material defined during thermal hydraulic coupled simulation. In general, most of Monte Carlo (MC) simulations typically employ the continuous energy representation of the neutron cross-section (XS) for all isotopes in the nuclear system. Therefore, in order to consider temperature feedback, i.e., Doppler broadening effect, during MC transport simulation, a large number ACE formatted XSs at various temperatures, i.e., 10~50K intervals, need to be pre-generated. This increases tremendous memory burden associated with storing the XSs during the neutron transport calculation.

In order to overcome the memory burden, various on-the-fly Doppler broadening techniques were proposed. One of the most novel approaches is the windowed multipole (WMP) representation which was proposed by Computational Reactor Physics Group (CRPG) in MIT [1]. This on-the-fly XS reconstructing method at the target temperature of interest significantly reduces memory burden from GB to several tens of MBs scale. In addition, the computational overhead of WMP representation is small in the overall Monte Carlo simulation.

In this paper, the concept and the idea from previous contribution related with the generation of WMP library for on-the-fly Doppler broadening is briefly reviewed. Then the application to UNIST in-house Monte Carlo code MCS [2, 3, 4] is introduced, and verification results for fuel pin problems are represented.

2. Methodology

This section briefly describes the methodology of the reconstruction of resolved resonance region XSs for on-the-fly Doppler broadening. In Sec. 2.1, the rigorous multipole representation and Doppler broadening techniques are summarized. The concept of WMP representation is described in Sec. 2.2 and the generation process of the WMP library is described in Section 2.3.

2.1 Rigorous multipole representation

Multipole representation is an alternative to the conventional R-Matrix theory to describe the microscopic XSs of different nuclides in the resolved resonance region. Hwang suggested its practical use and extended that concept for higher angular momentums, i.e., s-, p-, d-, f-wave resonances [5, 6]. Eqs. (1), (2), and (3) show radiative capture and fission, total, and elastic scattering reaction microscopic XSs, respectively, in terms of multipole resonance parameters. There are three main formalisms to convert the resonance parameters given in evaluated nuclear data files (ENDF) into multipole parameters: Single-Level, Multi-Level Breit-Wignet (SLBW and MLBW) and Reich-Moore (RM) formalism.

The main advantage of the given approach over the methods widely used to reconstruct the XS is the capability to apply analytical Doppler broadening. In other words, the resonance microscopic XS at any temperature of interest can be directly generated from the multipole parameters.

$$\sigma_{x=\gamma,f}(E)=\frac{1}{E}\sum_{l,J}\sum_{\lambda}^{N}\sum_{j=1}^{2(l+1)} \frac{\mathrm{Re}\left[R_{l,J,\lambda,j}^{(x)}\sqrt{\pi}W(z_0)-\frac{-iR_{l,J,\lambda,j}^{(x)}}{\sqrt{\pi}}C\left(\frac{p_{l,J,\lambda,j}^{*}}{\sqrt{\xi}},\frac{\sqrt{E}}{2\sqrt{\xi}}\right)\right]}{2\sqrt{\xi}}, \quad (1)$$

$$\sigma_t(E)=\sigma_p(E)+\frac{1}{E}\sum_{l,J}\sum_{\lambda}^{N}\sum_{j=1}^{2(l+1)} \frac{\mathrm{Re}\left[R_{l,J,\lambda,j}^{(t)}\sqrt{\pi}W(z_0)-\frac{-iR_{l,J,\lambda,j}^{(t)}}{\sqrt{\pi}}C\left(\frac{p_{l,J,\lambda,j}^{*}}{\sqrt{\xi}},\frac{\sqrt{E}}{2\sqrt{\xi}}\right)\right]}{2\sqrt{\xi}}, \quad (2)$$

and

$$\sigma_s=\sigma_t-\sigma_f-\sigma_\gamma, \quad (3)$$

where l,J are relative orbital angular momentum and total spin; λ,N are resonance index and total number of resonances; $R_{l,J,\lambda,j}^{(x)}, p_{l,J,\lambda,j}^{*}, E$ are residue corresponding to the reaction x, complex conjugate of the resonance pole, and energy, respectively. $z_0=\frac{\sqrt{E}-p_{l,J,\lambda,j}^{*}}{2\sqrt{\xi}}$; $\xi=\frac{k_bT}{4A}$; k_b is the Boltzmann`s constant; and T is the target temperature. Hwang noticed that correction factor

$C\left(\frac{p^*_{l,J,\lambda,j}}{\sqrt{\xi}},\frac{\sqrt{E}}{2\sqrt{\xi}}\right)$ is only significant at very low energies, and it can be neglected at higher energies [6].

As afore-mentioned, the multipole representation allows the production of XS at any temperatures directly from resonance poles and residues. Doppler-broadened line-shape functions $\psi-\chi$ are used to modify the XS with respect to the temperature [7]. It is based on the Faddeeva function as shown in Eq. (4).

$$W(z)=\frac{i}{\pi}\int_{-\infty}^{\infty}\frac{e^{-t^2}dt}{z-t}=\frac{2}{\sqrt{\pi}\theta}\left(\psi(x,\theta)+i\chi(x,\theta)\right), \quad (4)$$

where $z=x+i\theta$ is the complex variable.

In case of rigorous multipole approach, all the poles are used to reconstruct XS. A disadvantage of the rigorous method, due to the large number of parameters, is that the evaluation of Faddeeva functions for all the poles requires a significant amount of computational time.

2.2 Windowed multipole representation

Conventionally, a single energy point microscopic XS is generated using all the resonance parameters given in nuclear data file. In order to decrease the XS generation time at a single energy point, the smooth behavior of the single resonance at the locations far from its peak is used. A similar trend was noticed in case of multipole parameters. This was another important founding associated with the individual pole XS behavior. Poles with positive real parts exhibits resonance behavior at the resonance energy, while remaining counterparts have smooth contribution [8].

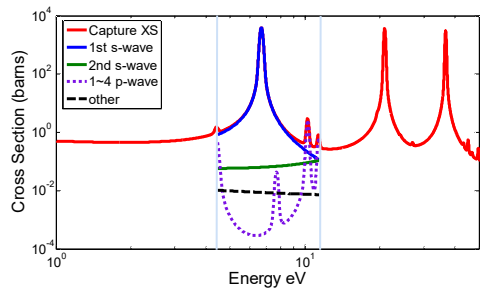


Fig. 1. Energy window for capture cross section of ^{238}U.

The peak and smooth contributions of fluctuating and non-fluctuation poles are presented in Fig. 1. As shown in Fig. 1, only fluctuating components make resonance behavior of the microscopic XS, and all the remaining components can be approximated using polynomial fitting. However, even though every single pole has smooth contribution far from its resonance peak, the summation gives very complicated background XS. This cannot be fitted by low order polynomial. In order to resolve the given issue, the energy window concept is used [9-11].

Basically, the resolved resonance energy range is divided into inner windows uniformly. In order to reconstruct the XS within the one particular inner window there required only fluctuating poles within and nearby their boundaries. The remaining poles give only smooth contribution which can be approximated by polynomial. Hence, on top of every inner window there is an outer window, which contains all important poles to reconstruct the resonance XS. This approach enables to decrease the number of poles used to reconstruct XS at every single energy point, and ignores the all non-fluctuating poles by applying low order polynomials. Fig. 2 shows the basic scheme of the window concept, with inner windows and corresponding outer windows. XSs constructed using the poles outside of the outer window are smooth and can be approximated.

Energy window concept also allows to minimize number of evaluations of Faddeeva function required for analytical Doppler broadening of microscopic XS at single energy point.

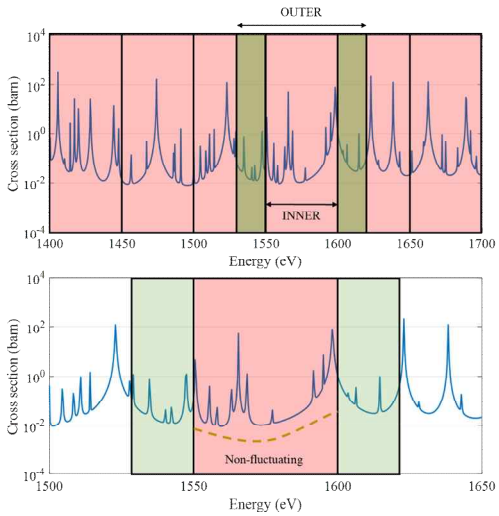


Fig. 2. Energy window concept scheme (inner and outer windows)

2.3 Windowed Multipole Library

There are several important parameters which need optimization in order to generate WMP library for the specific isotope satisfying with the XS error criteria. Inner and outer windows determine the number of poles used to reconstruct the temperature dependent XS at single energy point. The order of the fitting polynomial highly depends on the number of poles within the outer window and the error criteria which need to be met. Fig. 3 shows the scheme to obtain the optimized inner and outer window sizes, and the polynomial order for any given isotope.

```
Convert Resonance Parameters into Multipoles
Initial guesses for inner window and outer window size

do inner window size:
    do outer window size:
        arrange poles indices (i_low, i_up) for  every inner window
        do inner window index:
            generate XS within the given window using ONLY poles (i_low, i_up)
            obtain background XS at 300 K and 3000 K
            do polynomial order = 2 : MAX(order)
                fitting of the background XS
                if error < 0.1 %
                    break
            end do polynomial order
        end inner window index
    end do outer window
end do inner window size
```

Fig. 3. Windowed multipole library generation algorithm

3. Numerical results

This section provides a verification of UNIST in-house generated WMP library for 308 isotopes with ENDF/B-VII.1 XS library. Current status of WMP is summarized in Table I. Two single fuel pin-cell problems were selected from the VERA benchmark suite [12].

Table I: Summary of ENDF/VII.1 WMP library in MCS

Resonance parameters	Method	Number of isotopes (# of WMP library)
YES	SLBW	8 (6)
	MLBW	268 (250)
	RM	54 (52)
	RML	1 (0)
NO	Point-wise XS	92(0)
	Total	423 (308)

3.1 Verification of WMP library with PWR Fuel Pin

In the VERA benchmark specifications, among all the pin-cell problems, 1C of the 3.1wt.% UO_2 fuel, and 1I of 5% gadolinia rods are selected. Pin-cell problem 1C is representative of normal fuel pin cases at the hot full power condition, and the problem 1I contains gadolinia which is the burnable poison material of the benchmark problem.

The MCS depletion calculations of the selected fuel pins are performed using ACE XSs, and the on-the-fly Doppler broadening routine employing the WMP library. For the depletion calculation of pins 1C and 1I, 100,000 histories are employed per cycle, 20 inactive and 200 active cycles.

The isotope-wise number density difference is calculated at BOC, MOC, and EOC for pins 1C, and 1I. Important fission products, the burnable absorber, and actinides were selected to verify the WMP library. The Pin 1C and Pin 1I number density relative differences are illustrated in Fig. 4 and Fig. 5 for fission product and actinides, respectively.

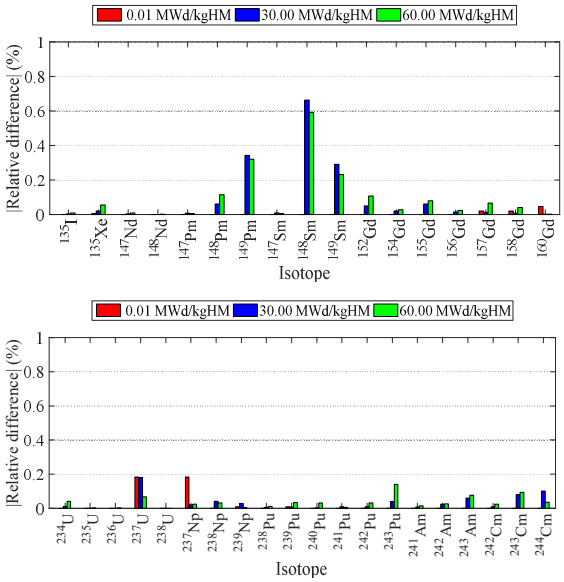


Fig. 4. Pin 1C relative differences in number density for fission product and actinides

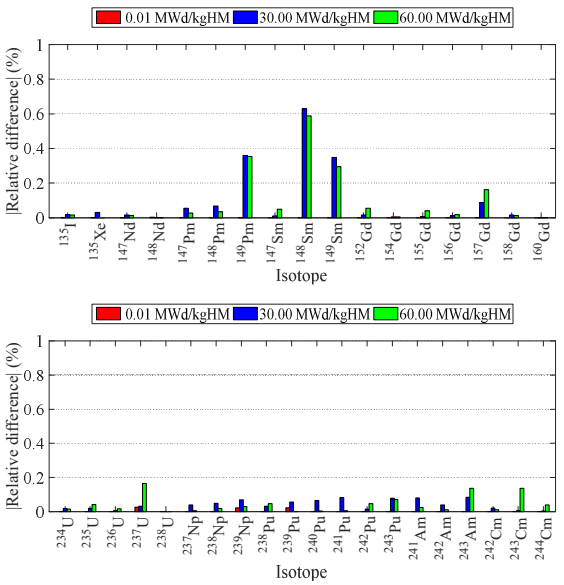
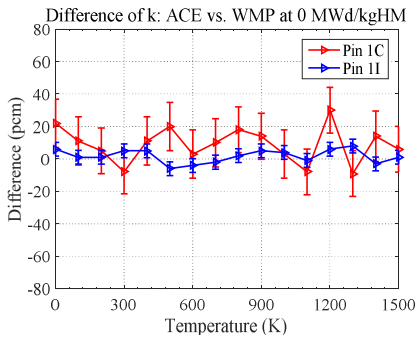


Fig. 5. Pin 1I relative differences in number density for fission product and actinides

The relative difference is less than 0.7 % for fission products, and 0.2 % for important actinides in both 1C and 1I pin-cell problems



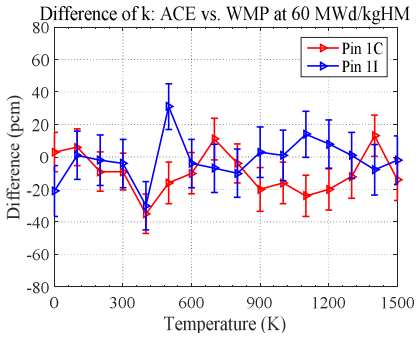


Fig. 6. Difference of k: ACE and WMP w.r.t. temperature at 0.00 and 60.00 MWd/kgHM

Next, the fresh and burned pins 1C and 1I are simulated at various temperatures starting from 0 K up to 1500 K.

The k_{inf} differences with corresponding standard deviations for pins 1C and 1I at 0.00 and 60.00 MWd/kgHM are illustrated in Fig 6 at various temperatures.

3.2 Performance test of WMP library

This section provides the performance tests result in terms of clock cycles for the WMP library application in on-the-fly Doppler broadening. The Monte Carlo code MCS contains a subroutine "get_xs_micro_all", which provides all the reaction XS types during the simulation. Within the given function, the temperature dependent XSs are from the ACE file, or the WMP reconstruction routine. The clock cycles are estimated per call of the subroutine. Table II shows the clock cycle comparison of the single temperature ACE XS utilization and on-the-fly Doppler broadening routine with the generated WMP library. Although the ACE XS lookup time decreased by 45 %, the overall performance of the subroutine decreases by 58 % due to on-the-fly XS generation. The slowing down of the subroutine providing the XS due to the WMP library contributes into a 28% performance loss of the MC simulation.

Table II: Estimated clock cycles per "get_xs_micro_all" call

	ACE	WMP	Difference (%)
Total	568	897	58%
ACE XS	84	46	-45%
WMP XS	-	284	-
Faddeeva*	-	130	-
Broadening polynomial*	-	5	-

* Sub-function

4. Conclusions

This paper presents a brief review of the methodology of WMP library generation and its application and verification in the on-the-fly Doppler broadening routine of MCS code. The conversion of conventional formalism resonance parameters into rigorous multipole parameters was performed. The reduction of the overall number of multipole parameters was achieved through the window concept. The verification of the generated WMP library was demonstrated by applying to VERA benchmark suite pin-cell problem using the Monte Carlo code MCS, in terms of multiplication factor and isotopic number density. The performance of the generated WMP library was evaluated. The XS generation time increases by 50 % and the overall Monte Carlo simulation performance loss is 30 %.

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