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

Calculating Resonance Parameter Sensitivity Coefficients in SCALE

Abdulla Alhajri,* Vladimir Sobes,† Chris Perfetti,† Benoit Forget,*

* *Department of Nuclear Science and Engineering, Massachusetts Institute of Technology*
† *Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN*
alhajri@mit.edu

Abstract - *Uncertainty in nuclear data constitutes one of the largest contributions to the uncertainty in our neutronic simulations. In order to be able to use the results from Monte Carlo codes, it is important that we are able to accurately, and efficiently calculate the uncertainties in reactor parameters arising from uncertainty in the nuclear data. We present here a method to propagate the nuclear data uncertainty via a sensitivity method that calculates the sensitivity to the resonance parameters, thereby remaining faithful to the physics. We show that this method is accurate, however it is not computationally efficient.*

I. INTRODUCTION

In recent years, uncertainty quantification has been coming under the spotlight in the nuclear science community. In particular, the propagation of uncertainty in nuclear data to calculated quantities for large systems, such as k_{eff}, reactivity coefficients, and peaking factors have been the focus of many research efforts. One of the most promising ways to propagate this uncertainty is the use of sensitivity methods. However all current approaches involve calculating the sensitivity to the cross sections and combining that information with the cross section covariance matrix. This paper shows that this method is not entirely faithful to the physics. We additionally propose calculating the sensitivity to the underlying resonance parameters. Our proposed methodology has been implemented in the SCALE 6.2 code package from ORNL[1]. The sensitivity coefficients have been validated using a direct perturbation benchmark. While the implementation is not yet complete, it offers a promising new way of faithfully propagating cross section uncertainty to calculated quantities.

II. NUCLEAR DATA UNCERTAINTY

Accurate evaluated nuclear cross section data are needed for radiation transport calculations for nuclear applications. In the cross section evaluation procedure, data evaluators attempt to fit the nuclear physics model to measured differential data by selecting and manipulating the resonance parameters that parametrize the formulation of the cross sections. The model, which can be derived from quantum scattering theory, results in an equation for the cross section of the form

$$\sigma(E) = f(E; \mathbf{\Gamma}) \tag{1}$$

where $\mathbf{\Gamma}$ are the resonance parameters. It is ultimately these resonance parameters that define the interactions of the nuclei[2]. The process of differential evaluation of the resolved resonance region is a mathematically overdetermined problem with no exact solution. Therefore, there is much choice left to the evaluator in seeking parameters that minimize a certain metric. Even once an evaluation is considered complete based on differential experimental data, it is not unique, and other possibilities exist that may satisfy the metrics used to determine the accuracy of the evaluation. Simply put, the experimentally measured cross section value at every energy point is reported only as a mean value and a standard deviation. Therefore, it is statistically equivalent for the cross section reconstructed from the resonance parameters, Γ, to pass above or below the mean experimental value by the same amount. This ambiguous choice previously has been left to the evaluator's discretion.

Much of the systematic uncertainty on differential cross section data comes from the normalization of capture and inelastic cross section measurements[3]. These measurements demand that the experimenter has a high degree of knowledge of the experimental flux; unfortunately, this is not always the case. In the best case, this results in larger uncertainties over certain energy regions of the experimental data. In the worst case, the experimental cross section data is misreported. This can be manifested in systematically larger or smaller mean values for the measured cross section or small uncertainty that does not reflect the actual state of knowledge. Unlike statistical uncertainty, systematic uncertainty can result in resolved resonance evaluations that produce a cross section that is too high over a large energy region. Therefore, the uncertainty on the normalization of experimental data is one of the biggest concerns in completing a new evaluation of a resolved resonance region based on differential experimental data.

When simulating the neutronics of a nuclear system, the uncertainty in the nuclear data constitutes one of the two major sources of uncertainty in the results of the simulation, the other being the errors introduced by the calculation scheme. The calculation scheme can effectively be driven to arbitrarily small values by either running more particles in Monte Carlo, or refining the phase space in a deterministic calculation. On the other hand, the uncertainties stemming from nuclear data cannot be reduced without revising the underlying nuclear data evaluations, and must thus be accounted for when conducting a reactor physics calculation. In the case of Monte Carlo neutronics calculations, which are often used as reference solutions for deterministic codes, nuclear data uncertainties propagated through the reactor core calculation make-up the bulk of the uncertainties. For instance, recent studies have shown that, in the case of the OECD/NEA Martin-Hoogenboom benchmark, the single propagation of ^{235}U, ^{238}U, ^{239}Pu cross section uncertainties and that of the H

and H_2O thermal scattering $S(\alpha,\beta)$ kernels yield local fission pin power uncertainties at mid-height ranging between 1% (in the center of the core) to 4% (at the periphery), while the statistical uncertainty of the Monte Carlo simulation was always well below 1% [4].

III. CURRENT SENSITIVITY METHODS

The current state of the art in nuclear data uncertainty propagation is based on the so called "sandwich formula." In this method, the cross section covariance matrix is sandwiched with the cross section sensitivity coefficients. The uncertainty, δR, in the quantity R can be expressed as

$$\delta R = S_\sigma^R C_{\sigma\sigma} S_\sigma^{R^T} \tag{2}$$

Where the sensitivity coefficient, S_σ^R is defined as:

$$S_\sigma^R = \frac{\partial R/R}{\partial \sigma/\sigma} \tag{3}$$

This sensitivity coefficient can be calculated in the MCNP [5], Serpent [6], and SCALE [1] codes using various methods such as IFP [7], CLUTCH [8], and the collision-history method [9].

1. Utilization of continuous energy Monte Carlo

The sensitivity, S_σ^R can be calculated using continuous energy Monte Carlo. However, in order to use the sandwich formula, the sensitivity has to be binned into an energy group structure. A finer group structure will approach the accuracy needed to fully reconstruct the continuous energy sensitivity profile, however this comes at the expense of drastically increasing the run time in order to achieve reasonable statistical convergence.

2. Treatment of temperature effects

Another issue with the present sensitivity methods is the use of the cross section covariance matrix, this matrix is dependant on the energy group structure, and temperature. The cross section covariance matrix is obtained from the resonance parameter covariance matrix by the following relation:

$$C_{\sigma\sigma} = \frac{\partial \sigma}{\partial \Gamma} C_{\Gamma\Gamma} \frac{\partial \sigma}{\partial \Gamma}^T \tag{4}$$

The resonance parameter covariance matrix, $C_{\Gamma\Gamma}$ is independent of temperature and energy group structure, however this is not the case for the derivatives $\frac{\partial\sigma}{\partial\Gamma}$. The derivatives must be Doppler broadened to an appropriate temperature, but the choice of such temperature is not obvious. In a system that contains multiple temperatures, the cross section covariance matrix can only be obtained for a single temperature, this leads to the unfortunate situation where the sensitivities, which correctly account for the temperature, are sandwiched with the covariance matrix, which is oblivious to the multiple temperatures.

IV. SIMILAR WORKS

As far as the authors are aware, only one study of the direct propagation of resonance parameter uncertainties has ever been done. This work was done by B. Morillon in 2000[10].

In that work, the neutron flux is expanded using a second order Taylor expansion with respect to the three resonance parameters that describe a single resonance $(E_\lambda, \Gamma_n, \Gamma_\gamma)$ giving the following expression:

$$\begin{aligned}\Delta\psi(\mathbf{r},\mathbf{\Omega},E) = &\frac{\partial\psi}{\partial E_\lambda}\Delta E_\lambda + \frac{\partial\psi}{\partial\Gamma_n}\Delta\Gamma_n + \frac{\partial\psi}{\partial\Gamma_\gamma}\Delta\Gamma_\gamma \\ &+ \frac{1}{2}\left(\frac{\partial^2\psi}{\partial E_\lambda^2}\Delta E_\lambda^2 + \frac{\partial^2\psi}{\partial\Gamma_n^2}\Delta\Gamma_n^2 + \frac{\partial^2\psi}{\partial\Gamma_\gamma^2}\Delta\Gamma_\gamma^2\right) \\ &+ \frac{\partial^2\psi}{\partial E_\lambda\partial\Gamma_n}\Delta E_\lambda\Delta\Gamma_n + \frac{\partial^2\psi}{\partial E_\lambda\partial\Gamma_\gamma}\Delta E_\lambda\Delta\Gamma_\gamma + \frac{\partial^2\psi}{\partial\Gamma_\gamma\partial\Gamma_n}\Delta\Gamma_\gamma\Delta\Gamma_n\end{aligned} \tag{5}$$

Morillon then shows that the derivatives of the flux can be expressed with the logarithmic derivatives of the transport and collision kernels, which in turn can be expressed using the derivatives of the cross section.

There are two drawbacks of this method. First, it requires the calculation of 9 derivatives for each resonance, hence this method does not scale well for larger problems. The other drawback is that the method only considers the elastic scattering reaction. The methodology presented in our work is capable of treating all reaction types, including fission.

This methodology is also able to treat the temperature effects by using the SIGMA1 procedure [11] to Doppler broaden the derivative of the cross section with respect to the resonance parameters. However, the SIGMA1 procedure has its own drawbacks, namely that it suffers from performance issues due to its large memory requirements, which leads to more cache misses.

V. METHODOLOGY

In order to properly treat the continuous energy nature of the problem, and to get away from the energy group structure, it is possible to rewrite the sandwich formula as such:

$$\delta R = S_\Gamma^R C_{\Gamma\Gamma} S_\Gamma^{R^T} \tag{6}$$

What we have done here is replaced the cross section covariance matrix with the resonance parameter covariance matrix. As previously mentioned, the resonance parameter covariance matrix is independent of the temperature and energy group structure.

The sensitivity to the resonance parameter can be written as:

$$S_\Gamma^R = \frac{\partial R/R}{\partial \Gamma/\Gamma} \tag{7}$$

By the chain rule, this can be expanded to

$$S_\Gamma^R = \frac{\partial R/R}{\partial \Gamma/\Gamma} = \frac{\partial R/R}{\partial \sigma/\sigma}\frac{\partial \sigma/\sigma}{\partial \Gamma/\Gamma} = S_\sigma^R \frac{\partial \sigma/\sigma}{\partial \Gamma/\Gamma} \tag{8}$$

The derivative, $\frac{\partial\sigma/\sigma}{\partial\Gamma/\Gamma}$, is analytic at $0K$, and the sensitivity S^R_σ is just the continuous energy sensitivity that is calculated by modern methods. The advantage of this method is that every continuous energy sensitivity that gets calculated in the code contributes to the sensitivity of all the resonance parameters at once, thereby allowing us to faithfully treat the continuous energy problem.

This new method was implemented in the SCALE 6.2 code package. In this implementation, the authors have demonstrated the ability to calculate the sensitivity of the eigenvalue, k_{eff}, to the resonance parameters, Γ. The cross section sensitivity, S^k_σ is calculated using the CLUTCH method [8]. The derivative of the cross section with respect to the resonance parameter, $\frac{\partial\sigma}{\partial\Gamma}$ is calculated using the AMPX code [12].

A flowchart of how the code is structured is included in Figure 1. It is clear from the flowchart that higher temperatures are treated in a structurally different way than the 0 K case, and therefore tested separately.

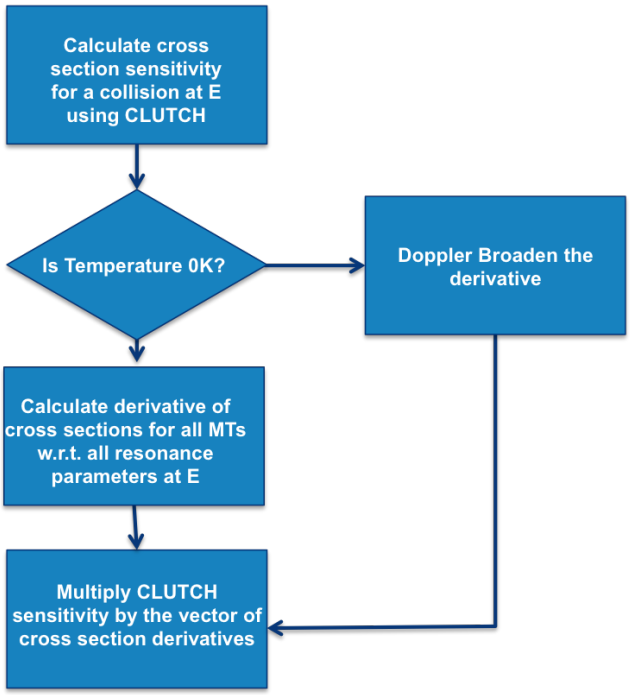

Fig. 1. Flow of the Resonance Parameter Calculation feature in SCALE

In the code, all the different reactions are treated separately, so the final output is the effect on the eigenvalue broken down by reaction type, which can be expressed as:

$$\frac{\partial k/k}{\partial\sigma_i/\sigma_i}\frac{\partial\sigma_i/\sigma_i}{\partial\Gamma_j/\Gamma_j}\ \forall i \in \text{Reactions}, \forall j \in \text{Resonance Parameters} \tag{9}$$

In order to get the final sensitivity of the resonance parameter we have to sum up all the contributions

$$\frac{\partial k/k}{\partial\Gamma_j/\Gamma_j} = \sum_{i\in rxns}\frac{\partial k/k}{\partial\sigma_i/\sigma_i}\frac{\partial\sigma_i/\sigma_i}{\partial\Gamma_j/\Gamma_j} \tag{10}$$

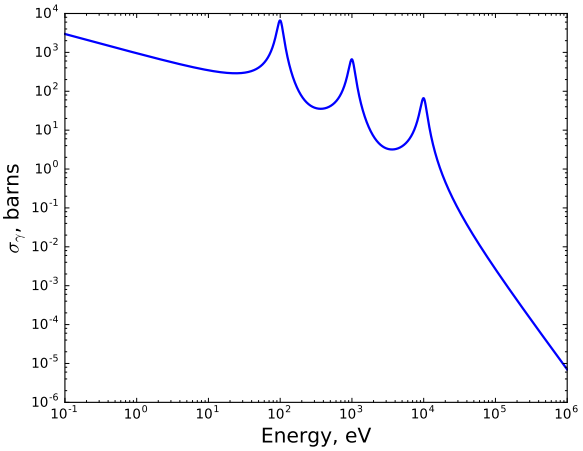

Fig. 2. Capture cross section of isotope X used in the benchmark

This is the result that we are after, it tells us the percentage change of the eigenvalue due to a percentage change in the resonance parameter.

VI. RESULTS AND ANALYSIS

The resonance parameter sensitivity method was implemented in SCALE and validated against a direct perturbation benchmark. The benchmark was an infinite homogeneous medium consisting of ^{235}U, ^{1}H, and a fictitious isotope (isotope X). Isotope X has three resonances at 100 eV, 1000 eV, and 10000 eV. The sensitivity to the resonance parameters of isotope X were calculated and the results are presented here.

Because of the differences in how the code treats 0 K cases and higher temperature cases, both cases were tested separately and presented here.

1. Zero Kelvin Case

As the name suggests, in this case, the temperature of the infinite homogeneous medium was set to 0 K.

It is clear, from the results, that the most sensitive resonance parameter is the location of the $1000\,eV$ resonance. From the value of the sensitivity [figure 3], we calculate that perturbing the resonance parameter by $8\,eV$ will result in a $100\,pcm$ change in the k_{eff}. In order to test this, four new fictitious isotopes were created with the second resonance appearing at $992\,eV$, $996\,eV$, $1004\,eV$, and $1008\,eV$. The isotope X was then replaced by each of the new perturbed isotopes and the problem was re-run. Plotting the change in the eigenvalue vs. the change in the resonance parameter, we can linearly fit the data, the slope of the fit should match the calculated sensitivity [figure 4].

A similar process was used to verify the results for the most sensitive neutron and capture widths, Γ_n and Γ_γ. The calculation validates the assumption of linearity for small perturbation in the resonance parameters. The result for the Γ_γ perturbation is presented in figure 5.

The uncertainty on the curve fit parameter was calculated

Resonance Parameter	Value [eV]	$\frac{\partial k/k}{\partial \Gamma/\Gamma}$	Uncertainty
E_1	100	0.034	0.000013
Γ_n^1	10	-0.033	0.000018
Γ_γ^1	10	-0.033	0.000041
E_2	1000	**0.129**	**0.000233**
Γ_n^2	100	-0.062	0.000019
Γ_γ^2	100	-0.062	0.000045
E_3	10000	0.093	0.000192
Γ_n^3	1000	-0.031	0.000013
Γ_γ^3	1000	-0.031	0.000026

Fig. 3. Result of the resonance parameter sensitivity calculation on isotope X

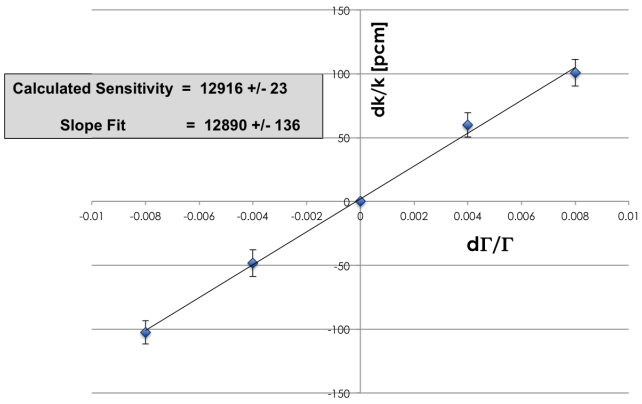

Fig. 4. The system with the perturbered E_2 was run through a Monte Carlo calculation, the results were then linearly fitted. The resulting fit had a slope that matched the calculated sensitivity

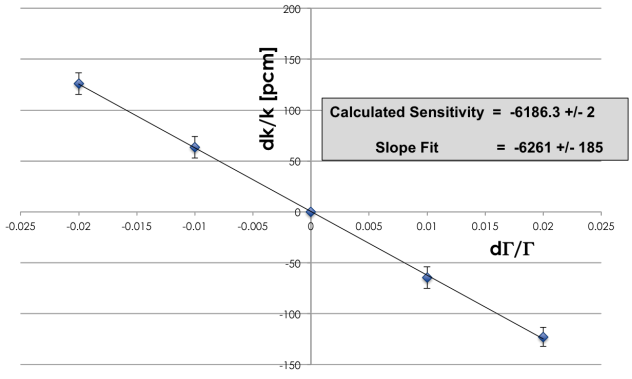

Fig. 5. The system with the perturbered Γ_γ was run through a Monte Carlo calculation, the results were then linearly fitted. The resulting fit had a slope that matched the calculated sensitivity

using a weighted linear least squares scheme. Each data point was assigned a weight that is inversely proportional to the variance calculated by the Monte Carlo run. The point at the origin had a weight of infinity since by definition, a 0% change in the resonance parameter will yield a 0% change in the eigenvalue. In our results, we see that the variance from the resonance parameter sensitivity calculation is much smaller than that from the least squares fitting, and that our results match up nicely.

One possible way to overcome the performance limitations of the Doppler broadening procedure would be to look at estimating the derivatives using a SLBW approximation to the cross section. Using this method would introduce errors that arise from the interference terms in the cross section, however the approximation will allow us to compute the derivatives much more efficiently.

2. Generalization to Higher Temperatures

In the previous section, we described how the resonance parameter sensitivity was calculated for a 0K benchmark. In order to generalize the method for higher temperatures, it is important to calculate the derivative of the Doppler broadened cross section, this can be mathematically posed as follows:

$$\frac{\partial \sigma_T}{\partial \Gamma} = \frac{\partial}{\partial \Gamma} \int S(E, E'; T) \sigma_{0K}(E') dE' \tag{11}$$

Where $S(E, E'; T)$ is the Solbrig kernel. Unlike in the 0 K case where the derivative of the cross section with respect to the resonance parameters can be obtained analytically, the derivative at higher temperatures must be computed numerically.

The structure of the Doppler broadening procedure as implemented in SCALE is shown in figure 6. This procedure turns out to be extremely time consuming. The rate limiting step is the second step, where an energy grid needs to be constructed in order to be able to reconstruct the Solbrig kernel within an allowable error. However, even when we manually over-ride that step, the procedure remains time consuming, making it almost impossible to produce any statistically meaningful results in a reasonable amount of time.

VII. CONCLUSION AND FUTURE WORK

There are two major takeaways from this work. The first is the confirmation that for small perturbations in the resonance parameters, the change in the eigenvalue is indeed linear and can be well approximated by the first derivative.

The second takeaway is that the resonance parameter approach is the most sensible way to propagate the uncertainty while still remaining faithful to the underlying physics. However, as we have shown here, this approach does not generalize well to higher temperatures.

The authors believe that in order to make this approach practical, it is possible to replace the R-Matrix formalism with the multipole formalism [13]. Thereby preserving the physics, while also making the higher temperature case faster to compute [14].

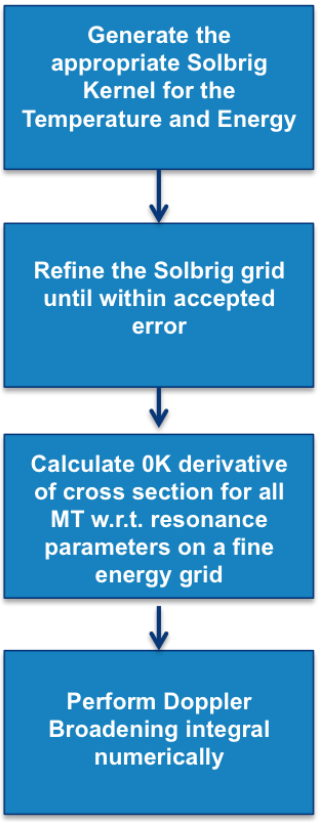

Fig. 6. Flow of the Doppler Broadening implementation in SCALE

REFERENCES

1. B. REARDEN, M. DUNN, D. WIARDA, C. CELIK, K. BEKAR, M. WILLIAMS, D. PEPLOW, C. PERFETTI, I. GAULD, W. WIESELQUIST, ET AL., "Overview of SCALE 6.2," Tech. rep., Oak Ridge National Laboratory (ORNL) (2013).
2. G. ARBANAS, V. SOBES, A. HOLCOMB, M. PIGNI, and D. WIARDA, "SAMMY: An R-matrix Bayesian Nuclear Data Evaluation Code,," in "The 2016 R-Matrix Workshop on Methods and Applications," (2016).
3. V. SOBES, L. LEAL, G. ARBANAS, and B. FORGET, "Resonance Parameter Adjustment Based on Integral Experiments," *Nuclear Science and Engineering*, **183**, *3* (2016).
4. S. C. VAN DER MARCK and D. A. ROCHMAN, "Nuclear data uncertainties for local power densities in the Martin-Hoogenboom benchmark," in "SNA+ MC 2013-Joint International Conference on Supercomputing in Nuclear Applications+ Monte Carlo," EDP Sciences (2014), p. 02410.
5. MCNP, "Monte Carlo Team, MCNPâĂŤa general purpose Monte Carlo N-particle transport code, version 5," Tech. rep., LA-UR-03-1987, Los Alamos National Laboratory, April 2003. The MCNP5 code can be obtained from the Radiation Safety Information Computational Center (RSICC), PO Box 2008, Oak Ridge, TN, 37831-6362 (5).
6. J. LEPPÄNEN, "SERPENT Monte Carlo reactor physics code," (2010).
7. B. C. KIEDROWSKI, F. B. BROWN, and P. P. WILSON, "Adjoint-weighted tallies for k-eigenvalue calculations with continuous-energy Monte Carlo," *Nuclear Science and Engineering*, **168**, *3*, 226–241 (2011).
8. C. M. PERFETTI and B. T. REARDEN, "Development of a generalized perturbation theory method for sensitivity analysis using continuous-energy Monte Carlo methods," *Nuclear Science and Engineering*, **182**, *3*, 354–368 (2016).
9. M. AUFIERO, A. BIDAUD, M. HURSIN, J. LEPPÄNEN, G. PALMIOTTI, S. PELLONI, and P. RUBIOLO, "A collision history-based approach to sensitivity/perturbation calculations in the continuous energy Monte Carlo code SERPENT," *Annals of Nuclear Energy*, **85**, 245–258 (2015).
10. B. MORILLON, "Resonance parameters perturbation with Doppler broadening in Monte Carlo neutron transport problems," *Annals of Nuclear Energy*, **27**, *1*, 21–42 (2000).
11. D. E. CULLEN and C. R. WEISBIN, "Exact Doppler broadening of tabulated cross sections," *Nuclear Science and Engineering*, **60**, *3*, 199–229 (1976).
12. N. GREENE, J. LUCIUS, L. PETRIE, W. FORD III, J. WHITE, and R. WRIGHT, "AMPX: A Modular Code System for Generating Coupled Multigroup Neutron-Gamma Libraries from ENDF/B," Tech. rep., Oak Ridge National Lab., Tenn.(USA) (1976).
13. R. HWANG, "A rigorous pole representation of multilevel cross sections and its practical applications," *Nuclear Science and Engineering*, **96**, *3*, 192–209 (1987).
14. C. JOSEY, P. DUCRU, B. FORGET, and K. SMITH, "Windowed multipole for cross section Doppler broadening," *Journal of Computational Physics*, **307**, 715–727 (2016).