

# Treatment of Neutron Resonance Elastic Scattering Using Multipole Representation of Cross Sections in Monte Carlo Simulations

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## Abstract

Predictive modeling and simulation plays a vital role in the design and licensing of nuclear reactors making it imperative that all physics interactions be represented as accurately as possible. In recent years, it was discovered that the kinematics of neutron resonance elastic scattering at high temperature were not fully accounting for the outgoing energy of neutrons. New methods were implemented in high-fidelity codes, like OpenMC being actively developed at MIT, to account for this phenomena. These methods rely on pre-tabulated cross section data. In parallel, advancements in cross section processing have brought research away from pre-tabulated data in an effort to properly account for temperature effects and reduce memory requirements. Both advancements have been separately and successfully implemented in OpenMC, but merging them poses a new challenge. This project will seek to develop an algorithm that can exploit the new data representation while still preserving the resonant scattering kinematics.

## I. Introduction

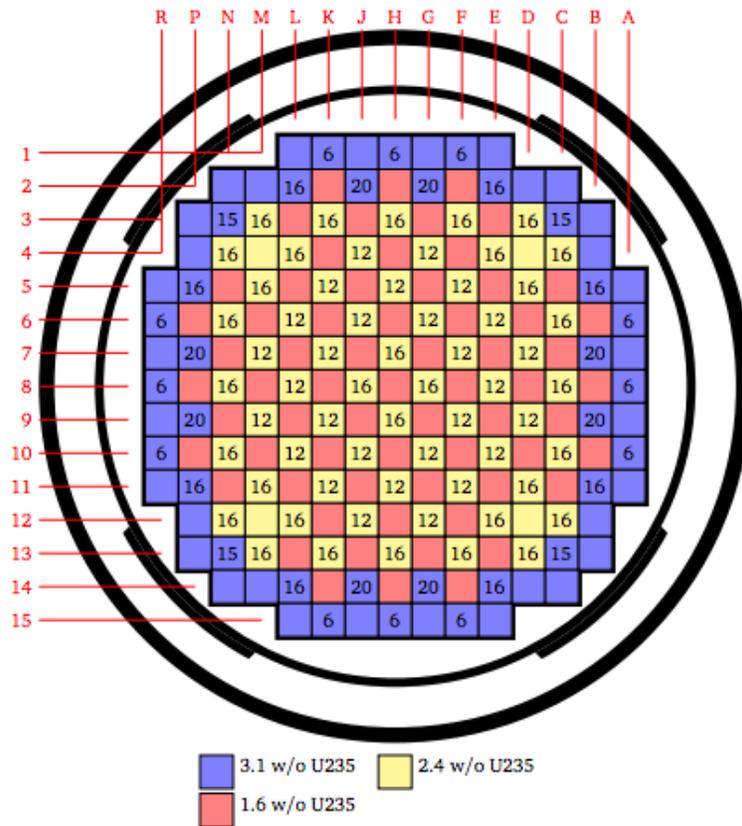
Simulations are vital to the safe design and operation of nuclear reactors, and they need to be able to accurately represent the physics of nuclear interactions. The resonance scattering phenomenon, in which the scattering cross sections of resonant nuclides can vary drastically within small energy intervals, is one such important physics consideration, as it can affect macroscopic values. This phenomenon was only discovered in 1991 (Sanchez), and its impact on reactor calculations, such as the fuel temperature reactivity coefficients, wasn't quantified until 10 years later.

Currently, methods to accurately treat resonance scattering are integrated with tabulated cross section values, which take up a significant amount of memory. It is desirable to minimize memory requirements and be able to calculate cross sections at any temperature desired for scalable high performance computing capable of multi-physics calculations. A new method for calculating cross section values on the fly with the Multipole algorithm has recently been implemented and verified in OpenMC, which is an open-source Monte Carlo particle transport code capable of modeling nuclear systems. The Multipole representation of nuclear cross sections reduce memory requirements up to a hundred fold, by storing only resonance parameters and then integrating to the values at whatever temperature desired. However, this method has not yet been used to treat resonance scattering,

nor has any other method on the fly cross section calculation,. It is the goal of this work to preserve the accurate kinematics of resonance scattering while reducing memory requirements with the Multipole cross section representation.

## II. Background

OpenMC is an open-source Monte Carlo neutron transport code that has been under active development at the Massachusetts Institute of Technology by the Computational Reactor Physics Group since early 2011 [1]. This code allows users to build models and run simulations of nuclear reactor cores and other nuclear systems, as shown in Fig. 1.



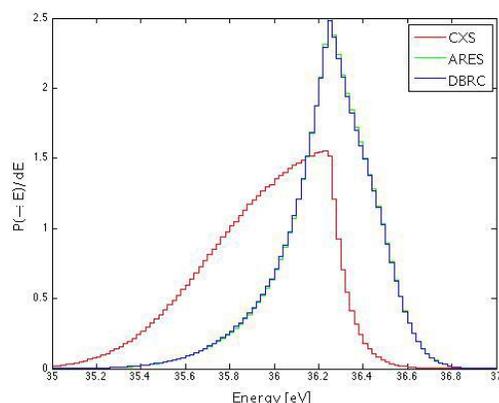
**Figure 1.** Layout of fuel assemblies, taken from BEAVRS full core benchmark, to demonstrate the modeling capabilities of OpenMC.

OpenMC has been shown to have excellent accuracy and scalability in criticality benchmark and full core eigenvalue calculations. OpenMC has been validated against several benchmarks in the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [2], the full core Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS) [3], and results obtained from MCNP [4]. OpenMC can be accessed online [5].

Correct treatment of the resonance elastic scattering is essential to the accuracy of reactor physics simulations. One verified way of correcting this assumption is the Doppler broadening rejection correction (DBRC) method [6], which has been implemented in OpenMC. This method samples a Maxwellian target velocity

distribution and performs rejection sampling on a 0 K scattering cross section. This rejection sampling can be extremely inefficient in the vicinity of resonances, leading to an increase in overall simulation runtimes.

A more efficient, recently developed method, the accelerated resonance elastic scattering kernel (ARES) sampling method [7], has also been implemented in OpenMC and shown to agree well with the Doppler broadening rejection correction method. ARES directly samples the 0 K scattering cross section distribution and then performs a rejection sampling of a Maxwellian distribution. The ARES method reduces the number of rejected values and consequently reduces the required computation time. Scattering kernels created from the DBRC and ARES methods are shown in Fig. 2.



**Figure 2.** The resonance scattering kernels for the 66.13 eV U-238 s-wave resonance for incident neutrons at 65.23 eV are plotted using three different methods, a constant cross section approximation (CXS), ARES, and DBRC. ARES and DBRC both produce accurate scattering kernels whereas CXS is a less accurate approximation.

At present, these two methods use tabulated, point-wise cross section data from the National Nuclear Data Center [8] in their sampling calculations. However, the multipole representation could drastically reduce memory requirements by 1-2 orders of magnitudes. The multipole representation was first proposed by Hwang [9], and it works by transforming resonance parameters into a set of poles and residues. Multipole representation has since been implemented in OpenMC, providing a simple way of computing nuclear data at any temperature, which is essential for multi-physics calculations. This approach also leaves a minimal memory footprint, which is essential for scalable high performance computing[10].

The mathematics and code behind the DBRC and ARES methods will need to be restructured and revised to incorporate the Multipole representation. However, we believe this can be done, and that doing so will enable further optimization of memory requirements and computational efficiency.

### III. Technical Approach

It is the goal of this work to preserve the accurate kinematics of resonance scattering while reducing memory requirements with the Multipole cross section representation. To do so, I will be studying the physics and mathematics behind the

multipole cross section representation and the DBRC and ARES methods. Because the ARES method works by directly sampling the 0 K scattering cross section distribution and then rejection sampling a Maxwellian distribution, it will need to be restructured to use the Multipole cross section representation rather than the actual cross section data. It is also possible that computational efficiency would be optimized by the reverse sampling tactic, ie. the DBRC method which directly samples the Maxwellian distribution of target velocities and then rejection sampling the Multipole representation of the 0K scattering cross sections. Both methods will need to be investigated.

The accuracy of the coupling of the DBRC/ARES and the Multipole algorithms will be verified. This will be done by comparing the effective multiplication coefficient obtained in the simulation outputs with the values obtained from simulating the same systems with the original tabulated cross section data. Comparisons will be made against the results determining optimal energy ranges to apply DBRC/ARES [11]. The results will be deemed accurate if the values fall within one standard deviation of the comparison values.

Runtimes and memory savings will be characterized in order to optimize their coupled implementation. These simulations will first be run for a single nuclide, which exhibits many resonances. U-238 is the obvious choice as it is the most abundant fuel element. Once this coupled approach has been verified for this nuclide, other nuclides can be investigated.

Once the code has been verified, further optimization of the computational efficiency can be investigated. This can be done for each resonance kernel by using a limited application of the resonance corrections over an optimal energy range rather than spanning the entire energy space. Similarly, the use of reactivity coefficients and runtimes will help in evaluating the optimization potential.

#### IV. Conclusion

It is the aim of this work to optimize memory requirements and computational efficiency in OpenMC's treatment of the resonance scattering phenomenon. This can be done through a coupling of the DBRC/ARES methods, which have been shown to accurately produce scattering kernels and model the kinematics of resonance scattering, and the Multipole algorithm, a mathematical way to represent nuclear cross sections that requires significantly less memory than a database of the actual cross sections. Key tasks and a schedule are shown in Table 1.

This is an exciting and active area of research in the nuclear reactor physics community, as OpenMC is under active development and is being used across various universities, laboratories and other organizations in the world. This project will give me a unique opportunity to advance recent work that is of practical interest to core designers and analysts. Furthermore, if significant optimization of the coupled method can be achieved, then a journal paper will be pursued in the spring semester. Regardless, the work has potential for a conference paper and presentation. It will also be a part of my senior thesis, and possibly a master's thesis if I choose to pursue the 5-year joint BS/MS program in Course 22.

## V. Timeline

Table 1 shows the proposed fall semester timeline for the project.

Table 1: Projected Timeline

October	- Install branch of OpenMC with Multipole cross section representation. - Learn Fortran
November	- Couple the ARES method with the Multipole representation of cross sections in the Fortran code - Run preliminary simulations of fuel pins using the coupled method for U-238 nuclide
December	- Complete and present poster of preliminary findings for 6.UAR - Conduct further simulations and optimizations
January	- Begin thesis writing and continue simulations and data gathering
February	- Finish analyzing data, complete first draft of thesis
March/April	- Complete thesis

## References

1. P. K. ROMANO and B. FORGET, "The OpenMC Monte Carlo Particle Transport Code," *Annals of Nuclear Energy*, **51**, 274, (2013).
2. NEA Nuclear Science Committee, 2009, "International Handbook of Evaluated Criticality Safety Benchmark Experiments," NEA/NSC/DOC(95)03, OECD Nuclear Energy Agency (2009).
3. N. HORELIK, B. HERMAN, B. FORGET, and K. SMITH, "Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS)," Proc. International Conference on Mathematics and Computational Methods Applied to Nuclear Science & Engineering (M&C 2013), Sun Valley, ID, May 5-9, (2013).
4. X-5 Monte Carlo Team, 2008, "MCNP – A General Monte Carlo N-Particle Transport Code, Version 5," LA-UR-03-1987, Los Alamos National Laboratory (2008).
5. P. K. ROMANO, "GitHub – Reactor Physics Benchmark Models," <https://github.com/mit-crpg/benchmarks>, accessed Feb. 11, 2015.
6. W. ROTHENSTEIN, "Neutron scattering kernels in pronounced resonances for stochastic Doppler effect calculations," *Annals of Nuclear Energy*, **23**, 441, (1996).
7. J. A. WALSH, B. FORGET, and K. SMITH, "Accelerated sampling of the free gas resonance elastic scattering kernel," *Annals of Nuclear Energy*, **69**, 116, (2014).
8. M. HERMAN, "Evaluated Nuclear Data File (ENDF) Retrieval & Plotting," National Nuclear Data Center, <http://www.nndc.bnl.gov/sigma/index.jsp>, accessed Feb. 15, 2015.
9. R. N. HWANG, "A rigorous pole representation of multilevel cross sections and its practical applications," *Nuclear Science Engineering*, **96**, 192, (1987).

10. B. FORGET, S. XU, and K. SMITH, "Direct Doppler broadening in Monte Carlo simulations using the Multipole representation," *Annals of Nuclear Energy*, **64**, 78, (2013).

11. V. TRAN and J. WALSH, "Impact of neutron resonance elastic scattering energy intervals on nuclear reactor reactivity calculations," Proc. American Nuclear Society Student Conference, College Station, TX, April 9-11, (2015).

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