On-the-Fly Nuclear Data Processing Methods for Monte Carlo Simulations of Intermediate and Fast Spectrum Systems

by
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Abstract

Computational methods for on-the-fly representation and processing of nuclear data within Monte Carlo neutron transport simulations of intermediate and fast spectrum systems are developed and implemented in a continuous-energy Monte Carlo code. First, a capability to compute temperature-dependent unresolved resonance region (URR) cross sections directly from zero-temperature average resonance parameters is presented. The use of this capability in benchmarking both evaluated and processed URR data is demonstrated. Results of this benchmarking lead to a partial resolution of a longstanding discrepancy between experiment and calculation results for a well-known fast critical assembly. Next, an on-the-fly probability table interpolation scheme for computing temperature-dependent URR cross sections is developed and used in analyses which show that interpolation on a relatively coarse temperature mesh (>100 K) can be used to reproduce results obtained with cross sections generated at an exact temperature. This enables the simulation of systems having detailed temperature distributions using probability table data which require significantly less memory than data generated on a fine temperature mesh. Additional methods for use in the investigation of two common approximations that are made in representing URR cross section data are developed. Namely, a multi-level URR cross section calculation capability is used to show that level-level interference effects in elastic scattering cross sections are negligible in many cases of interest. A capability to generate resonance structure in competitive reaction cross sections is used to show that neglecting cross section structure for reactions other than elastic scattering, capture, and fission can lead to non-negligible, unconservative biases (>100 pcm) in criticality safety calculations. The principal underlying assumption of the probability table method is also tested by comparing the results it yields with results that are averaged over many independent simulations, each using a single,
independent realization of URR resonance parameters. Unknown URR resonance structure is observed to induce an uncertainty on the multiplication factor for intermediate and fast spectrum systems that is nearly an order of magnitude greater than that which is purely stochastic. This significantly increases the uncertainty to which results of simulations of those systems should be stated. Finally, a procedure for consistent, on-the-fly sampling of temperature-dependent neutron reaction kernels which requires no additional secondary distribution data is presented. It is used to show that Doppler effects may have only a small impact on elastic scattering secondary angular distributions at typical power reactor operating temperatures but can be appreciable at astrophysical temperatures.

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Chapter 1

Introduction

In the context of neutron transport simulations, the arbitrarily complex physics and geometrical models enabled by Monte Carlo methods [1] are extremely desirable features. In fact, continuous-energy Monte Carlo codes such as MCNP [2], MC21 [3], Serpent [4], and TRIPOLI [5] are widely regarded as the gold standard for the simulation of particle transport in nuclear systems. However, historically, the computing resources available for these simulations were only sufficient to run Monte Carlo codes as benchmarking tools or for criticality safety calculations; detailed reactor physics calculations were intractable. With the increased processing power and memory capacity of modern high-performance computing (HPC) systems, though, Monte Carlo simulations are increasingly being considered for full-core reactor analysis [6, 7].

Many advanced reactor technologies — including the majority of the designs proposed through the Gen IV Initiative [8], traveling wave reactors, and resource-renewable boiling water reactors — rely on neutron spectra that range from epithermal to fast. High-fidelity, computationally efficient simulations of both the reactors themselves, and also the critical assemblies that are utilized to obtain relevant nuclear data are required for reactor design, licensing, and operation. For this reason, efforts to research, develop, and eventually deploy these technologies will benefit from improved
computational methods for the analysis of systems with intermediate and fast neutron spectra.

In order to accurately and efficiently simulate fast reactor systems, there is a need for developing methods that take better advantage of Monte Carlo’s allowance of highly complex physics models and that reduce the floating-point operations and/or memory burdens associated with these detailed modeling capabilities. On-the-fly Monte Carlo nuclear data processing methods provide an opportunity for improved physics and computational efficiency in simulations of intermediate and fast spectrum systems. The development and analysis of computational methods for the improved modeling of cross sections and secondary angular distributions in Monte Carlo simulations of intermediate and fast spectrum systems is the focus of this thesis research. Section 1.1 will outline the methods that are developed and the principal contributions of this work. The remainder of the chapter contains more detailed discussions of the specific types of nuclear data that are relevant to reactor simulations in Section 1.2, computational methods that have been developed previously to represent and process these data for Monte Carlo simulations in Section 1.3, and the computational methods for nuclear data processing developed in this research in Section 1.4.

1.1 Principal Contributions

The unresolved resonance region (URR) encompasses those intermediate incident neutron energies, between the resolved resonance and fast energy regions, at which individual resonances cannot all be resolved experimentally even though distinct structure exists in nature. With precise cross section values unknown at any specific energy in the URR, representation of resonance structure must instead rely on average URR resonance parameters and theoretical statistical distributions of those parameters [9].
Computational methods for calculating URR resonance cross sections on-the-fly within Monte Carlo neutron transport simulations are developed in Chapters 2 and 3. Results demonstrating their use as benchmarking tools for both evaluated and processed nuclear data are provided. These results

- lead to a partial resolution of a longstanding discrepancy between experiment and calculation results for a well-known fast critical assembly and

- show that coarse temperature mesh interpolation of probability table data is suitable for the simulation of systems having detailed temperature distributions.

Alternate approaches for representing URR cross section data are presented in Chapters 4 and 5. They are used in analyses which test three key approximations that are typically employed when modeling URR resonance structure. These results

- provide quantitative justification for the widespread assumption that level-level interference effects in URR elastic scattering cross sections are negligible,

- show that neglecting cross section structure for reactions other than elastic scattering, capture, and fission can lead to non-negligible, un-conservative biases (>100 pcm) in criticality safety calculations, and

- demonstrate that unknown URR resonance structure can induce uncertainties in multiplication factor results which are significantly greater than the purely stochastic uncertainties that are typically stated.

Another challenge in processing nuclear data for use in continuous-energy Monte Carlo neutron transport codes is the treatment of secondary angular distribution data. This is especially true in modeling intermediate and fast spectrum systems
which have appreciable neutron populations at the energies at which these distributions can vary rapidly with energy. Further complicating the matter are the Doppler effects which arise from the thermal motion of target nuclei. Typically, the temperature dependence of secondary angular distributions is entirely neglected except at energies where the distributions are actually largely energy-independent. A procedure for consistently treating the effects of non-zero nuclear velocities on cross sections, scattering kinematics, and angular distributions is developed in Chapter 6. Results computed using this procedure show that

- Doppler effects can have a strong impact on secondary angular distributions in elastic scattering events at astrophysical temperatures.

1.2 Nuclear Data in Reactor Simulations

The high-fidelity simulation and analysis of reactor systems requires capabilities to represent a variety of nuclear data. That is, data which describe the relevant nuclear physics phenomena that occur within a reactor must be represented in order to simulate the system.

The nuclear data needed for describing the physical processes that must be modeled in reactor simulations are derived from evaluated nuclear data files. Each file is the product of an evaluation, the term for the process that nuclear scientists go through when compiling the best possible knowledge of the nuclear data for a single nuclide into a single file that is self-consistent\(^1\) and complete.\(^2\) As such, an evaluated file is an amalgamation of experimental data, theoretical nuclear model calculations, and adjustments of data to integral benchmark experiments. The ENDF-6 format \([10]\) is the near-universally accepted specification for the structure of an evaluated file,\(^3\)

\(^1\)In practice, consistency between all nuclear data in an evaluated file is not achieved, although inconsistency can be reduced to a negligible level.

\(^2\)Completeness is judged relative to the needs of the evaluated file's end-users' application (e.g., reactor physics calculations).
Table 1.1: Selected evaluated nuclear data file libraries

<table>
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<tr>
<th>Evaluated Nuclear Data Library</th>
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<td>JENDL-4.0 [17]</td>
<td>Japan Atomic Energy Agency [18]</td>
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<td>CENDL-3.1 [21]</td>
<td>China Nuclear Data Center [22]</td>
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<td>RUSFOND-2010 [23]</td>
<td>Institute of Physics &amp; Power Engineering [24]</td>
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<tr>
<td>BROND-2.2 [25]</td>
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though some laboratory-specific formats, such as ENDL [11], are still in use and efforts to develop a modern, flexible format are currently being pursued under the Generalized Nuclear Data (GND) format project [12].

Evaluated nuclear data files for different nuclides are collected into evaluated nuclear data libraries. The production of these libraries is performed at the national and international levels with several different countries and organizations issuing their own data. There is often significant overlap between the nuclear data contained in the various libraries. For reference, Table 1.1 lists common libraries alongside their parent organization.

Two specific types of nuclear data which are of particular importance to the simulation of fission reactor systems are neutron cross sections and secondary neutron distributions. Brief reviews of each type are provided in Sections 1.2.1 and 1.2.2, respectively.

### 1.2.1 Cross Sections

A microscopic cross section, conventionally denoted by $\sigma$, is proportional to the probability per differential element of an incident particle’s flight path that the particle will interact with some target particle in a particular way. The constant of proportionality that makes this relationship hold is the volumetric number density of target
particles, \( N \). Macroscopic cross sections, conventionally denoted by \( \Sigma \), are simply the product of \( N \) and \( \sigma \) and give the aforementioned probability. Common units for \( N \), \( \sigma \), and \( \Sigma \) are atoms/cm\(^3\), cm\(^2\), and cm\(^{-1}\), respectively. A unit known as a *barn* [b] is often used when stating microscopic cross sections and is equal to \( 10^{-24} \) cm\(^2\).

The way in which cross sections are defined depends on the level of detail needed to describe the interaction between particles. For instance, there are *total* cross sections to describe the probability of any interaction occurring and there are *partial* reaction cross sections to describe the probability of a particular interaction taking place. There are also *integrated* cross sections, which give the probability that an interaction will end in some general region of phase-space, and *differential* cross sections for giving the probability that an interaction will end in some more specific region of phase-space. These notions become more concrete when viewed through the lens of an application in which cross sections are used.

For reactor physics simulations, in which modeling the interactions of neutrons with nuclei is the chief concern, cross sections which describe neutron-nucleus interactions are needed. As discussed in the sections below, neutron cross section behavior can exhibit significant dependence on the energy of the incident neutron. For this reason, further discussion of neutron cross sections, and the associated nuclear data, will be divided into explanations of the thermal, resolved resonance, unresolved resonance, and fast energy regions in Sections 1.2.1.1 to 1.2.1.4, respectively.

### 1.2.1.1 Thermal Region

When a neutron is in thermal equilibrium with the material in which it exists, it is considered a *thermal neutron*. There is no absolute energy requirement for a neutron to be thermal, except that it is in thermal equilibrium with its surroundings. In the parlance of reactor physics, though, the thermal energy region refers to energies neighboring that of a thermal neutron in a reactor system that is near operating
temperatures. In this context, energies below a few eV are typically considered thermal.

In this region, neutron energies are comparable to the chemical binding energy of the atoms in a lattice or individual molecule. This means that the individual target nuclei cannot be accurately modeled as a free gas. Also, the neutron wavelength is comparable to the inter-atomic spacing between nuclei in a lattice or molecule which results in diffraction effects as the neutron, viewed as a wave, passes through a medium of identical molecules. These phenomena lead to complex variations in energy-dependent scattering cross sections that are tightly coupled to material properties [26].

Thus, chemical region may be a more appropriate term for characterizing such energies [9].
Additionally, the well-known $1/v_n$ cross section dependence, with neutron velocity, $v_n$, is present at all temperatures, even 0 K, in the absorption cross section and becomes more pronounced at higher temperatures as can be deduced from Figure 1.1 which shows the $^{238}$U capture cross section at both 0 K and $10^7$ K.

For the elastic scattering cross section, the $1/v_n$ variation is not present at 0 K but emerges at non-zero temperatures when cross sections are averaged over a distribution of target velocities. This is evident in Figure 1.2 which shows the $^1$H elastic scattering cross section at both 0 K and 900 K.
1.2.1.2 Resolved Resonance Region

At incident neutron energies above the thermal region, a compound nucleus can form with high probability if the combined energy of the neutron-nucleus system aligns with an energy level of the compound nucleus. The high probabilities of compound nucleus formation lead to peaks in the neutron cross section values at these energies [27]. Such peaks are referred to as resonances. The sharp structure associated with individual levels (i.e., resonances), which can be seen in the total cross section for $^{238}$U at 293.6 K in Figure 1.3, must be carefully accounted for in neutron transport simulations [28].

![Figure 1.3: $^{238}$U total cross section at 293.6 K](image)

The resolved resonance region (RRR) corresponds to incident neutron energies where the resonances for a given nuclide are pronounced and well-separated from neighboring
resonances. These properties make individual resonances more easily distinguishable from one another in cross section measurement experiments. That is, the resonances can be resolved experimentally. Once experimental data is obtained, nuclear data evaluators perform a fitting procedure to determine the energies and partial widths, collectively known as resonance parameters, of individual resonances. SAMMY is one commonly used code for fitting resonance parameters to experimental data via Bayesian updating techniques [29]. The resulting resonance parameters are the primary component of RRR nuclear data that are stored in an evaluated nuclear data file. Then, the RRR parameters can be used to reconstruct energy-dependent cross section values for transport simulations.

1.2.1.3 Unresolved Resonance Region Cross Sections

The intermediate incident neutron energies between the RRR and fast energy region make up the unresolved resonance region (URR). These energies are those at which individual resonances cannot all be resolved experimentally even though, in nature, each resonance exhibits distinct structure, just as in the RRR. This is due to decreasing energy resolution with increasing incident energy in neutron cross section measurement experiments — such as is caused by finite chopper thickness, path length, and target sample size in a typical time-of-flight setup. With precise cross section values unknown at any specific energy in the URR, representation of resonance structure must instead rely on average resonance parameters and theoretical statistical distributions of those parameters [9].

The URR can be visualized in the plot of the 293.6 K $^{239}$Pu total cross section in Figure 1.4. It is apparent that there is a discontinuity in the representation of the cross section at 2.5 keV. This is the energy at which individual resonances were determined by evaluators to be unresolvable and the RRR ends; and the start of the URR, where cross sections are often displayed as an average value. Each nuclide with a URR evaluation in the ENDF/B-VII.1 library is listed along with its URR energy
bounds in Appendix A.

Figure 1.4: $^{239}\text{Pu}$ total cross section at 293.6 K

For nuclides with similar masses, the precise bounds of URR energy intervals will differ due to differences in nuclear level densities; a higher density of energy levels in a compound nucleus will cause resonances to become unresolvable at lower energies. This can be seen in Figure 1.5 which shows that, relative to $^{238}\text{U}$, $^{235}\text{U}$ exhibits the URR phenomenon at a lower energy due to its resonances being more closely spaced in energy which necessitates an average cross section representation.

The calculation of the averaged URR cross section requires average resonance parameters throughout the URR. This requires the determination of averages of resonance parameter values (i.e., resonance energies and partial widths) which are, by definition, unknown in the URR. A simplistic approach is to simply take the parameter averages over the resonances at the upper energies of the RRR and use those values for URR
Figure 1.5: $^{238}$U and $^{235}$U total cross sections at 293.6 K

calculations. However, this neglects the energy dependence of the average resonance parameters above the RRR. In order to obtain average resonance parameters at energies that are actually within the URR, a fit of experimental data using equations of statistical level theory, as introduced by Wolfenstein [30] and further developed into the Hauser-Feshbach formulae [31], can be performed, and average resonance parameters that would yield the observed data are extracted. This is the procedure employed by the FITACS code [32] which has also been incorporated as a module of SAMMY.

However, the smoothed, energy-averaged cross sections computed from averaged parameters can differ significantly from the values generated in a single realization of structured resonance cross sections. Figure 1.6 displays these two representations of the $^{238}$U total cross section in the URR at a temperature of 293.6 K.
Figure 1.6: Averaged and structured $^{238}\text{U}$ URR total cross sections at 293.6 K

Faithfully accounting for URR resonance structure becomes especially important in the simulation of fast spectrum systems which typically have an appreciable neutron flux at energies within the unresolved regions of their constituent nuclides. If adequate models and processing methods are not used to reconstruct resonance structure in the URR, reaction rates will be mis-predicted, often resulting in unconservative effective multiplication factor calculations.

1.2.1.4 Fast Region

At sufficiently high incident neutron energies ($\sim$0.5 MeV), the nuclear reaction mechanism transitions from being purely due to the formation and decay of a compound nucleus to a pre-equilibrium mode in which the incident neutron penetrates the nu-
ucleus, undergoes some interaction with neighboring nucleons, and is emitted prior to full equilibration of the neutron-nucleus system [33]. Neutron cross sections at these energies can be calculated with theoretical nuclear model codes that account for pre-equilibrium processes such as GNASH [34], TALYS [35], and EMPIRE [36]. Reactions at still higher energies (∼5 MeV) are dominated by a direct reaction component whereby the incident neutron interacts with just a few nucleons in its immediate vicinity before exiting the nucleus. Optical model cross section calculations [37] become viable in this regime.

At these energies individual resonances become very broad and are spaced close enough together in energy that they overlap significantly with one another. The localized cross section structure of a single resonance is insignificant relative to the broad structures, known as Ericson fluctuations [38], which encompass several resonances over a wide energy range. The energies that are characterized by this sort of cross section behavior comprise the fast energy region. Much as the onset of both RRR and URR cross section behavior are nuclide-dependent, the threshold for what can be considered the fast energy region will vary for different nuclides with the boundary typically coming at lower energies (∼0.1 MeV) for heavier resonant nuclides than for lighter ones.

1.2.2 Secondary Distributions

In order to specify a particle-target interaction with the detail required by a typical continuous-energy Monte Carlo transport code, secondary particle distributions must be known. That is, the phase-space for each particle that exists in the simulation after the occurrence of an interaction needs to be determined. As the locations of all outgoing particles are already fixed at their interaction sites, this amounts to determining the post-interaction direction and energy of each particle. The distributions that describe the secondary particle directions and energies, and the manner in which these distributions are represented as nuclear data, are discussed in Sections 1.2.2.1
1.2.2.1 Angular Distributions

The direction of an outgoing particle is given by a secondary angular distribution. For each type of neutron-nucleus interaction that is to be considered, there is a distribution that describes the probability of a secondary neutron exiting the interaction with a given direction. In practice, these probability distributions are almost always given in terms of the cosine of the angle between the pre-interaction and post-interaction particle direction vectors. With the incident neutron direction and the cosine rotation known (once it is sampled), the secondary particle energy can be calculated or sampled from another distribution depending on the interaction type and available data.

The corresponding neglect of any azimuthal asymmetries in secondary direction probabilities is typically an accurate assumption at neutron energies most-encountered in fission systems (<20 MeV). In fact, the secondary neutrons from many compound nucleus interactions, including fission, \((n, 2n)\), and some inelastic scattering, are simply treated as being emitted isotropically. However, elastic scattering distributions are typically treated with anisotropy in scattering cosine and, though used rarely, some provisions for azimuthal asymmetry are made by the ENDF-6 format [10].

Elastic scattering cosine distributions depend on the incident neutron energy and are given in either the center-of-mass or laboratory frame of reference, more commonly the former. They can be represented in a variety of ways including tabulated data or coefficients for Legendre polynomial expansions which are then converted into discrete tabular distributions. Alternatively, using the formalism of Blatt and Biedenharn [39], detailed angular distributions can be reconstructed directly from resonance parameters.
To illustrate some of the characteristics that are commonly found in these distributions, the probability of a neutron elastically scattering from $^{239}$Pu with a given center-of-mass scattering cosine is shown in Figure 1.7. It can be noticed that the secondary angular distribution for elastic scattering changes depending on the energy of the incident neutron.

![Figure 1.7: $^{239}$Pu elastic scattering secondary angular distribution](image)

At the lower energies more often encountered in the softer spectra of highly-moderated systems such as light-water reactors (LWRs), the secondary distribution is largely isotropic. Moving to the higher energies which are more frequently encountered in fast reactors, significant forward-peaking is observed. In order to correctly predict system leakage, which can be a particularly important quantity due to its role in reactivity feedback mechanisms commonly employed in fast reactor designs [40], an accurate representation of this peaking, and secondary angular distributions, in general, is
However, while there is a definite observable preference for forward-peaked secondary neutrons at higher incident energies, the variation of the scattering cosine distribution in Figure 1.7 is relatively smooth across energies. This is a feature of secondary distributions that are calculated from theoretical nuclear models that do not account for the energy level structure of the compound nucleus. When this structure is accounted for, a detailed secondary distribution which exhibits resonance structure in the energy variable across individual levels is observed. This is evident in Figure 1.8 which displays the secondary angular distribution for elastic scattering from $^{56}$Fe as calculated directly from resonance parameters.

Figure 1.8: $^{56}$Fe elastic scattering secondary angular distribution
1.2.2.2 Energy Distributions

Just as the directions of post-interaction secondary neutrons must be defined in order for the transport simulation to proceed, so too must the secondary energies. For both elastic scattering and inelastic scattering to discrete energy levels, these outgoing energies can be calculated directly using the scattering cosine; the reaction threshold energy, if applicable; and kinematic equations. Distributions must be given, though, for reactions such as fission, \((n, 2n)\), and inelastic scattering to a continuum of levels.

Secondary neutron energy distributions are given by a variety of expressions, known as laws in the ENDF-6 format. Among the ENDF-6 laws are tabulated energy-probability data; exponential and generalized evaporation spectra [41]; a Maxwellian fission spectrum, an extension to the evaporation spectra [42]; a Watt spectrum [43]; and a Madland-Nix fission spectrum, a systematics-based (i.e., semi-empirical) formulation [44].

1.2.2.3 Correlated Energy-Angle Distributions

In somewhat more complex neutron-nucleus interactions (e.g., those involving charged particles or a continuum of levels) or if more detailed information about an individual interaction is required (e.g., correlation between emitted particles or the state of the recoil nucleus), it may not be possible to sample the cosine by which the particle’s flight path is rotated and then directly calculate an outgoing energy (as in elastic or level inelastic scattering), or even to sample separate distributions for angle and energy independently. These cases can require the sampling of secondary distributions for both a cosine of direction change and outgoing energy in a correlated fashion. That is, the angular distribution to be sampled is dependent on the value sampled, first, from an energy distribution, or vice versa. As with the secondary energies, there is a set of laws which are used to specify the coupled distributions. The ENDF-6 manual
documents each of these representations [10].

1.3 Computational Methods for Nuclear Data Processing

The field of nuclear data processing encompasses the procedures employed to transform evaluated nuclear data files to applied nuclear data libraries that can be used in transport codes. These procedures take the form of the computational methods that are implemented in production nuclear data processing codes such as NJOY [45], PREPRO [46], AMPX [47], CALENDF [48], and FUDGE [49]. The thrust of the research presented in this thesis is the development and analysis of improved computational methods for modeling URR cross sections and secondary distributions in Monte Carlo codes. Common methods currently used for cross section processing are described briefly in Section 1.3.1 and those used for processing secondary distribution data are described in Section 1.3.2.

1.3.1 Cross Sections

Among the most important types of nuclear data required for neutron transport simulations are cross sections. These values characterize the frequency with which various neutron-nucleus interactions occur. For example, in the course of a simulated neutron’s random walk, they are used to sample the distance between interaction sites and also the type of interactions that occur at each site. However, in order to obtain cross section values in a form suitable for use within a transport code, it is necessary to perform a series of pre-processing procedures on the evaluated nuclear data discussed in Section 1.2.1. This section gives brief explanations of the primary nuclear data processing methods used to prepare continuous-energy neutron cross
sections for use in Monte Carlo transport simulations.

1.3.1.1 Scattering Law Tables

In the thermal energy region, typically up to a few eV, where the effects of chemical binding between atoms and wave diffraction effects become appreciable, tables of cross section data which give secondary angular and energy distributions, and their associated probabilities, are required. These tables describe the thermal scattering law for a particular nuclide as it behaves in a particular material. The thermal scattering law may also be denoted as simply $S(\alpha, \beta)$ which indicates its dependence on a variable derived from the dimensionless momentum transfer of an interaction, $\alpha$, and on another variable derived from the dimensionless energy transfer, $\beta$. With $\alpha$, $\beta$, and some additional material properties, tables of double-differential cross sections and probabilities can be generated at discrete energies and temperatures. This typically amounts to generating data at $\sim10$'s of discrete energies and temperatures for power reactor applications [50]. However, sampling techniques exist which allow these tables to be treated as continuous distributions in both energy [51] and temperature [52]. The LEAPR and THERMR modules of NJOY are often employed for the task of generating the $S(\alpha, \beta)$ data to be used in Monte Carlo codes.

1.3.1.2 Resonance Reconstruction

In the resolved resonance region, continuous-energy cross sections consisting of linearly interpolable tabulated energy-cross section pairs must reflect the resonance structure of cross sections as a function of energy. The generation of these cross sections directly from resonance parameters is known as resonance reconstruction. The resonance reconstruction process proceeds by utilizing the resonance parameters — resonance energies and partial reaction widths — from an evaluated nuclear data file in a collection of formulae derived from R-matrix theory [53], known as a resonance
formalism, which then yields cross section magnitudes. There are several different resonance formalisms, each one of which makes a different set of approximations to the mathematically rigorous R-matrix theory and, as a result, these formalisms reproduce the cross sections observed in nature with varying degrees of fidelity. Among the most common resonance formalisms are single-level Breit-Wigner (SLBW) [54] which assumes a single, isolated resonance; multi-level Breit-Wigner (MLBW) which extends SLBW to account for interference between levels; Adler-Adler [55] which is a multi-level formalism primarily suitable for fissile nuclides; and Reich-Moore [56], a more rigorous multi-level formalism which accounts for interference between neutron reaction channels.

The basic computational method required to process the evaluated nuclear data (i.e., resonance parameters) into continuous-energy cross sections is simply a correct implementation of the analytical equations for the desired resonance formalism. Various levels of complexity are then introduced when parameters such as error tolerance are considered. Separate absolute allowable errors on cross section magnitudes and resonance integrals are common checks to ensure that cross sections are generated with sufficient accuracy but also on an energy grid that is not unnecessarily dense. The RECONR module of NJOY is an example of a resonance reconstruction tool.

1.3.1.3 Doppler Broadening

Resonance parameters are a property of the nucleus, and thus do not have a temperature dependence. Evaluated nuclear data files may therefore be thought of as providing 0 K resonance parameters. From these parameters, energy-dependent neutron cross sections can be reconstructed, also at 0 K. However, in a material at non-zero temperature, the thermal motion of target nuclei creates a range of relative energies between the incident neutron and target nucleus. This range of relative energies creates a range of attainable cross section values.
Neutron transport simulations typically require cross section values that are a function of the incident neutron energy. In order to account for the range of possible cross section values arising from thermal target motion, an averaging process, known as *Doppler broadening*, must be performed to get a single, *effective* cross section value at each tabulated energy point that characterizes the range of all possible values. The objective of this averaging is to obtain effective cross sections that preserve temperature-dependent reaction rates in transport simulations.

A widespread Doppler broadening methodology assumes that target nuclei behave as an ideal gas at the temperature of the material in which they reside. Then, the 0 K cross section is convolved with a distribution of target velocities that are isotropic in direction and obey a Maxwell-Boltzmann distribution of speeds. When resonance parameters are used in the SLBW, MLBW, or Adler-Adler formalisms, this convolution can be performed analytically via use of the $\psi - \chi$ integrals [57], symmetric and asymmetric Voigt profiles. However, if cross sections deriving from Reich-Moore parameters are desired, additional computational methods are required. The convolution integral can be performed with numerical kernel broadening methods such as SIGMA1 [58] or a finite-difference diffusion approach [59]. Pointwise cross sections derived from SLBW, MLBW, or Adler-Adler parameters are also amenable to broadening with these two methods. Alternatively, resonance parameters provided for use in the SLBW, MLBW, Adler-Adler, or Reich-Moore formalisms can be converted to pole parameters [60] which can then be used in a general pole representation which allows for analytical Doppler broadening [61]. Thorough reviews of Doppler broadening theory and solution methods can be found elsewhere [62, 63].

1.3.1.4 Probability Tables

In order to more faithfully account for resonance structure and the resulting energy self-shielding effect in the URR — a phenomenon that can be worth hundreds of pcm$^4$

$^4$1 *per cent mille* (pcm) is a common unit of reactivity equivalent to 0.00001.
in intermediate spectrum systems — the probability table method was proposed [64].
This method relies on the sampling of discrete cross section values with associated
discrete probabilities such that, in the limit of many samples, the expected cross
section value at a given incident neutron energy is preserved. Although expected cross
sections are preserved, there is a distribution of discrete cross section magnitudes and
it is this distribution that provides a more realistic model for URR self-shielding.

Probability tables are generated in a pre-processing step before the start of a neutron
transport simulation. In general, a different set of tables is required at every tempera-
ture, for each nuclide with a URR in a simulation. Certain practical considerations in
implementing the probability table method are well-documented [65, 66, 67, 63].

1.3.2 Secondary Distributions

The methods by which secondary distributions are to be reconstructed are prescribed
in evaluated nuclear data files. Reconstruction of elastic scattering cosine distribu-
tions, for example, involves either simply reading in tabulated distributions pro-
vided by evaluators or converting the Legendre polynomial expansions generated from
evaluator-supplied coefficients into discretized distributions typically containing ∼10’s
of points. The results are secondary distributions, as functions of incident neutron
energy, for a stationary target. At this time, all production nuclear data processing
codes which treat secondary distribution data — both angular and energy — employ
a zero-temperature assumption. That is, thermal target motion is neglected and the
0 K secondary distributions are provided to neutron transport codes. Nuclear data
processing codes do not produce temperature-dependent secondary distributions for
transport codes to sample because methods for Doppler broadening the 0 K distribu-
tions do not exist [45].

Now, within the transport code, once an interaction location, interacting nuclide,
and reaction have all been sampled, the velocity of the target nucleus is implicitly
neglected when sampling secondary distributions, subject to certain exceptions. This results in the sampling of distributions at some other energy than the true relative energy between the neutron and target nucleus where the secondary distributions may be different.

1.4 Research Objectives

Because several advanced reactor technologies, including gas-cooled, lead-cooled, and sodium-cooled reactor designs, rely on fast neutron spectra, improvements in the accuracy of evaluations of certain types of nuclear data and in the methods of treating these data in simulations are likely to see increased interest in coming years. Primarily, this thesis examines methods for treating two types of nuclear data that are especially relevant to simulations of fast spectrum systems. These are URR neutron cross section data and post-reaction secondary neutron distributions (e.g., elastic scattering cosine probabilities). In this section the computational methods that are developed in this thesis to process these data are introduced. All of the methods are implemented in the continuous-energy Monte Carlo neutron transport code OpenMC [68]. URR cross section processing methods are discussed in Section 1.4.1 and methods for processing secondary distribution data are discussed in Section 1.4.2.

1.4.1 Unresolved Resonance Region Cross Section Treatments

A precisely known cross section value for reaction $x$ can be written as a Lebesgue integral in terms of a Dirac $\delta$-function in $\sigma'_x$-space such that

$$\sigma_x(E_n) = \int_{-\infty}^{\infty} d\sigma'_x \delta(\sigma'_x - \sigma_x(E_n)) \sigma'_x.$$  (1.1)
This is, though, just a special instance of a more general case in which the distribution of $\sigma'_x$ values — each of which corresponds to one of the possible cross section realizations — cannot be collapsed to a precise value with a $\delta$-function. Though precise cross section values at any given incident neutron energy, $E_n$, in the URR are unknown, the probability distribution of cross section values, $P(\sigma'_x \mid E_n)$, can be constructed from mean unresolved resonance parameter values and the statistical distributions of those values which are derived under the assumption that the Hamiltonian of a nucleus can be described by a random matrix with normally distributed elements [69]. An expression for the expected cross section value can then be written as

$$\langle \sigma_x(E_n) \rangle = \int_{-\infty}^{\infty} d\sigma'_x P(\sigma'_x \mid E_n)\sigma'_x. \tag{1.2}$$

This averaged, expected value is equivalent to an energy-averaged, infinite-dilute cross section. Historically, in the absence of precisely known URR resonance structure, these infinite-dilute cross sections were used in Monte Carlo neutron transport simulations.

Use of the infinite-dilute cross sections, though, is tantamount to neglecting the effect of energy self-shielding. In obtaining expected cross section values in the manner just described, the resonance structure of the URR is smoothed out. That is, in the narrow energy intervals where resonances actually occur, there is a reduced value and in the wider energy intervals between real URR resonances, there is an increased value. So, over the majority of URR energies, infinite-dilute cross sections are greater than the unknown, precise values. Thought of in terms of dilution, the averaged cross sections will not produce the flux depression that is observed in the vicinity of a resonance, as illustrated in Figure 1.9, that occurs under finite-dilution conditions.

The resulting over-prediction of flux leads to the over-prediction of reaction rates. It is known that these over-predicted reaction rates, notably capture by resonant absorbers (e.g., $^{238}\text{U}$), can be significant in simulations of fast and intermediate spectrum
systems. This can result in under-predicted, unconservative $k_{\text{eff}}$ eigenvalue calculations [70]. The probability table method [64] was developed in order to stochastically account for URR resonance structure and mitigate the undesirable effects associated with the use of infinite-dilute cross sections. The methods for modeling URR resonance structure that are investigated in this thesis are introduced in Sections 1.4.1.1 to 1.4.1.4.

1.4.1.1 Direct Cross Section Calculation

The first area of research to be explored is on-the-fly generation of URR cross sections in Monte Carlo neutron transport simulations — with the term on-the-fly referring to methods which perform the calculation of some value within the simulation itself, rather than those which utilize values that are pre-computed prior to the initialization of a simulation. The on-the-fly treatment will allow a continuous representation of
the energy, temperature, and cross section magnitude variables. This is in contrast to the probability table method which requires discrete sets of cross sections and corresponding probabilities at discrete energy points for discrete temperatures. Also, the method will be able, as an option, to account for or neglect the resonance structure of competitive reaction cross sections. This will enable straightforward quantification of the bias introduced in simulation results by the common practice — which is prescribed by the ENDF-6 format — of neglecting the fine structure in all such cross sections.

With on-the-fly methods for the $S(\alpha, \beta)$ thermal scattering energy region [52] and the resolved resonance energy region [71, 72, 73] already demonstrated, and the relatively sparse pointwise data that is sufficient to describe the fast energy region, the URR is the remaining computational bottleneck with respect to the computer memory required for storing neutron cross section data. The computational efficiency of simulations will be improved with an on-the-fly URR cross section calculation capability through a reduction of the memory burden associated with URR cross section data. Currently, in simulations having detailed temperature distributions, production codes require the storage of probability tables for every nuclide with a URR at several discrete temperatures. Rather than requiring the storage of probability tables, the on-the-fly method depends on only temperature-independent average resonance parameters which amount to just a few kilobytes of memory per nuclide.

The method relies on the statistical generation of a URR cross section realization which consists of resonance parameters, sampled from theoretical distributions, about the required energy (i.e., the incident neutron energy). Once a localized realization of resonance parameters is generated, temperature-dependent cross sections can be calculated via the SLBW or MLBW formalism and the $\psi-\chi$ integrals. This can be repeated at each event that requires URR cross section values within a Monte Carlo simulation. The on-the-fly URR cross section calculation method is presented in Chapter 2.
1.4.1.2 Probability Table Interpolation

In order to realize some of the memory reduction benefits associated with the direct, on-the-fly method for calculating URR cross sections without significantly increasing runtime, a probability table interpolation scheme is investigated. The method proceeds, as a pre-processing step, by generating a three-dimensional mesh in the energy, temperature, and cross section magnitude variables. This mesh is generated in such a way that the cross section magnitudes are equiprobable across all energy-temperature pairs. This allows cross section magnitudes to be sampled and interpolated consistently within a transport simulation. The methods for generating probability tables and then interpolating on-the-fly are presented in Chapter 3.

1.4.1.3 Alternate Resonance Data Representations

With the notable exception of CALENDF [48], virtually all nuclear data processing codes — and consequently, all Monte Carlo neutron transport codes — follow the ENDF-6 standard of an SLBW resonance cross section representation in the URR. The shortcomings of the SLBW representation, such as the possibility of negative elastic scattering cross section values at energies near resonance-potential scattering interference dips and its neglect of interference between energy levels, are well-known and documented [10].

This portion of the research will involve the use of a multi-level resonance formalism, namely the ENDF-6 version of MLBW, for the representation of URR cross sections. This formalism makes fewer approximations to the rigorous R-matrix theory and, in concordance, does not suffer from the aforementioned inadequacies to the same extent as the SLBW formalism. In Chapter 4, differences between energy-dependent cross section values computed with both SLBW and MLBW formalisms are investigated, as are the tally results from simulations in which each formalism is used.
The current state-of-the-practice method of employing the SLBW resonance formal-
ism, using ENDF-6 format data, for URR cross section calculations has the side effect
of restricting the energies over which resonance structure can be treated thoroughly
to those below the second threshold reaction energy for a given nuclide. This is be-
cause only a single competitive partial reaction width, which usually corresponds to
the first-level inelastic scattering reaction, is allowed in the ENDF-6 format. When,
at a sufficiently high incident neutron energy, the channel for the next-highest energy
threshold reaction is opened, the ENDF-6 SLBW resonance parameter data can no
longer describe all possible reactions. For this reason, at the second reaction threshold
energy, the URR treatment is often terminated and the pointwise fast energy region
cross section data begins. Further, to avoid even the possibility of having to treat
multiple open competitive reaction channels, the ENDF-6 standard prescribes that
all competitive reaction cross sections are to be represented with pointwise data in
the URR.

This is problematic because, at these energies, energy resolution in cross section
measurement experiments is so poor that only very broad cross section structure
spanning several resonances is discernible in pointwise data. The aim of this research
topic is to accurately model the resonance structure of the first threshold reaction
for energies at which its channel is the only one that is open. Simulations using this
representation are then used to quantify the biases in calculated results that are due
to the approximate representation of fine structure competitive reaction cross sections
with smoothed pointwise data. These results are found in Chapter 4.

1.4.1.4 Independent Resonance Realizations by Simulation

The generation of URR cross section realizations corresponding to single, independent
sets of resonance parameters sampled from the theoretical distribution functions, and
subsequent use of these individual realizations in independent Monte Carlo simula-
tions is detailed in Chapter 5. This process differs from the event-based on-the-fly
and probability table procedures in which a new cross section realization is to be generated at the incident neutron energy each time that a cross section is needed within the simulation. Using the cross section values corresponding to a single URR realization throughout a simulation does away with the unphysical assumption that any new cross section value is entirely independent of all cross section values previously calculated in the simulation.

The use of single, independent URR cross section realizations in independent Monte Carlo simulations allows for the computation of the true expected tally values. It also allows for the determination of the variance of possible results about that expected value. This gives the uncertainty that is an unavoidable consequence of a lack of knowledge of the true cross section resonance structure that exists in nature. The use of a single URR realization also offers memory savings relative to a pointwise representation in energy and/or a fine temperature mesh because cross section values will still be calculated on-the-fly from temperature-independent resonance parameters.

It should be noted that a mean result obtained over many independent simulations is merely an expected value. The true result will not be obtained unless the true resonance ensemble that exists in nature is stochastically generated, which would require the generation of an infinite number of realizations. It is also worth noting that the estimate for the expected value of a result, a value that is obtained by taking the mean over independent simulations, will not be equivalent to the corresponding result obtained from a single simulation with event-based realizations in which a new resonance set is generated about each new incident neutron energy. Correlation between the cross section values calculated at two or more successive neutron events is irrevocably lost through the generation of independent realizations at the different energies.
1.4.2 Secondary Distribution Doppler Broadening

Production-level nuclear data processing codes produce secondary angular distributions that are temperature-independent; they are equivalent to 0 K distributions. As a result of this, and because no methods have been developed to correct for it within Monte Carlo simulations, production-level transport codes do not correctly treat secondary angular distributions in the presence of thermal target motion.

To eliminate this longstanding approximation, a new method for on-the-fly Doppler broadening of secondary angular distributions — one which requires only the 0 K distributions that nuclear data processing codes already produce — is derived, implemented, and tested for elastic scattering in Chapter 6. Results which quantify some of the effects of the stationary target assumption are presented.
Chapter 2

Direct Cross Section Calculation

2.1 Background

In recent years, reliance on cumbersome legacy nuclear data preparation procedures and the computer memory required to represent continuous-energy neutron cross sections have been reduced by promising methods for on-the-fly processing of thermal scattering data [52] and resolved resonance region (RRR) cross sections [71, 72, 73]. However, the treatment of unresolved resonance region (URR) data has received less attention. A high-fidelity, memory-reducing, on-the-fly method for generating URR neutron cross sections in continuous-energy Monte Carlo transport simulations is the focus of this chapter. With this method, each time that a cross section value is needed within the simulation, a realization of unresolved resonance parameters is generated about the desired energy and temperature-dependent single-level Breit-Wigner (SLBW) resonance cross sections are computed directly via use of the analytical $\psi$-$\chi$ Doppler integrals. Because the calculation proceeds directly from temperature-independent average URR resonance parameters, significant memory reductions relative to discrete-temperature probability table treatments are possible. The capability is demonstrated to be a flexible tool for benchmarking both evaluated
and processed nuclear data. An explanation of the method’s implementation, analysis of results, and conclusions are given in Sections 2.2 to 2.4, respectively.

2.2 Implementation

In this section the process for on-the-fly generation of URR cross sections in the continuous-energy Monte Carlo neutron transport code OpenMC [68] is described. The sampling of unresolved resonance parameters and use of the sampled parameters in cross section computations using the SLBW formulae are discussed in Sections 2.2.1 and 2.2.2, respectively.

2.2.1 Level Spacings and Partial Widths

In the energy region about any incident neutron laboratory system energy, $E_n$, at which it is necessary to compute a realization of URR cross section values, an ensemble of resonances must be stochastically generated. This ensemble, sometimes referred to as a resonance ladder in the context of probability table generation, is determined by the energies at which resonances occur as well as the partial reaction widths characterizing each of the resonances. The process for sampling these values proceeds directly from the unresolved resonance parameters given in File 2 of an ENDF-6 format [10] evaluated nuclear data file.

Mean unresolved resonance parameter values are given for each of the individual spin sequences, which are defined by an orbital angular momentum quantum number, $l$, and a total angular momentum quantum number, $J$. There are $N_l$ orbital quantum numbers associated with the URR for a given nuclide. For each of these $N_l$ values, there are $N_J(l)$ total angular momentum quantum numbers. That is, $N_l$ is a nuclide-dependent quantity and $N_J(l)$ is dependent on both the nuclide and the $l$ values for
that nuclide.

For each \((l, J)\) spin sequence, level spacings (i.e., differences between adjacent resonance energies) and partial reaction widths are sampled using those parameters’ mean values and their statistical distributions. The mean parameter values at a specific \(E_n\) are determined by interpolation\(^1\) between the values at the energies tabulated in File 2. The statistical distributions of level spacings and partial reaction widths are given by the Wigner probability density function (PDF) and \(\chi^2\) PDFs with varying numbers of degrees of freedom, respectively \([74, 75]\). The Wigner distribution for level spacings is written as

\[
P_W \left( \frac{D^{l,j}(E_n)}{\langle D^{l,j}(E_n) \rangle} \right) = \frac{\pi D^{l,j}(E_n)}{2\langle D^{l,j}(E_n) \rangle} \exp \left( -\frac{\pi D^{l,j}(E_n)^2}{4\langle D^{l,j}(E_n) \rangle^2} \right).
\] (2.1)

A trivial inversion of the resulting cumulative distribution function (CDF) allows the direct sampling of a level spacing,

\[
D^{l,j}(E_n) = \langle D^{l,j}(E_n) \rangle \sqrt{\frac{-4 \log (\xi)}{\pi}},
\] (2.2)

with a random number on the unit interval, \(\xi\). Figure 2.1 displays both sampled and analytical representations of the distribution.

Partial widths for reaction \(r\), \(\Gamma_r\), are obtained by sampling a \(\chi^2\) distribution,

\[
P_{\chi^2(\mu_r)}(y) = \frac{\exp \left( -\frac{y}{2} \right) y^{\mu_r - 1}}{2^{\mu_r/2} \Gamma \left( \frac{\mu_r}{2} \right)};
\] (2.3)

\[
y \equiv \mu_r \frac{\Gamma_r^{l,j}}{\langle \Gamma_r^{l,j}(E_n) \rangle},
\]

\(^1\)A nuclide-dependent interpolation scheme is prescribed in an ENDF-6 file.
with a reaction channel-dependent number of degrees of freedom, \( \mu_r(l, J) \). The \( G(\frac{\mu_r}{2}) \) term in (2.3) is the Gamma function,

\[
G\left(\frac{\mu_r}{2}\right) = \int_0^\infty x^{\frac{\mu_r}{2}-1}e^{-x}dx.
\] (2.4)

As implemented, Equation (2.3) is transformed into a distribution which is amenable to a trivial sampling procedure, i.e., a discrete PDF with equiprobable nodes each having a probability
\[ \int_{y_{i-1}}^{y_i} P_{\chi^2(\mu_r)}(y')dy' = \frac{1}{N}; \]

\[ i = 1, 2, ..., N; \]

\[ y_0 = 0; \]

\[ y_N \to \infty \]

and a value given by

\[ \langle y'_i \rangle = N \int_{y_{i-1}}^{y_i} y' P_{\chi^2(\mu_r)}(y')dy'. \] (2.6)

Using a sample \( y \) along with the mean parameter values and degrees of freedom provided in an ENDF-6 file, it is straightforward to sample partial widths for fission, \( \Gamma^{l,J}_f \), and the single competitive reaction, \( \Gamma^{l,J}_x \), by rearranging Equation (2.3). In the case of radiative capture, it is assumed that \( \mu_\gamma \to \infty \). This results in Equation (2.3) approaching a Dirac \( \delta \)-function (and a probability of unity) for \( \Gamma^{l,J}_\gamma = \langle \Gamma^{l,J}_\gamma \rangle \). The energy-dependent sampled neutron width is calculated as

\[ \Gamma^{l,J}_n(E_n) = \nu_l(E_n) \sqrt{E_n} \langle \Gamma^{l,J}_n,0 \rangle \mu_n \frac{\Gamma^{l,J}_{n,0}}{\langle \Gamma^{l,J}_n \rangle} \] (2.7)

using the mean reduced neutron width value, \( \langle \Gamma^{l,J}_{n,0} \rangle \), given in an ENDF-6 file. The derived variables \( \nu_l \) and \( \rho \) are given by \( P_l/\rho \) and \( a_c k(E_n) \), respectively. In these expressions, \( k \), \( a_c \), and \( P_l \) are the center-of-mass neutron wavenumber, channel radius, and orbital quantum number-dependent penetration factor, respectively.
The wavenumber is given by

$$k(E) = \frac{10\sqrt{2m_n}}{\hbar c} \frac{A}{A + 1} \sqrt{|E|}$$  \hspace{1cm} (2.8)

with $m_n$, $\hbar c$, and $A$ being the mass of a neutron in eV, the reduced Planck constant multiplied by the speed of light in eV-fm, and the ratio of the mass of the target nucleus to that of a neutron, respectively.

The channel radius is related to the scattering radius, $a_s$, which is to be treated as energy-dependent, or not, if the NRO ENDF-6 flag is 1 or 0, respectively. For a scattering radius that is independent of energy, a NAPS ENDF-6 flag set to 0 indicates that the channel radius should be calculated as

$$a_c = 0.123 \times A^{1/3} + 0.08.$$  \hspace{1cm} (2.9)

In this case, $a_c$ should be used in the computation of penetrabilities, $P_l$, and shift factors, $S_l$, whereas $a_s$ should be used to calculate hard sphere phase shifts, $\phi_l$. If the NAPS flag is set to 1, $a_s$ should be used in determining the penetrabilities, shift factors, and phase shifts.

For a scattering radius that is dependent on energy, as in the energy-independent case, NAPS set to 0 indicates that $a_c$ is to be computed with (2.9) and used in the penetrabilities and shift factors with $a_s$ being used in the hard sphere phase shifts. If NAPS is set to 1 or 2, the penetrabilities, shift factors, and phase shifts are all calculated using $a_s$. However, in the case that NAPS is set to 2, an energy-independent $a_s$ is given and should be used for $P_l$ and $S_l$. Expressions for $P_l$, $\phi_l$, and $S_l$ are given in the next section.
2.2.2 Single-level Breit-Wigner Cross Sections

From the sampled level spacings and partial reaction widths, cross section values at a given $E_n$ are computed using a so-called many-level Breit-Wigner model\textsuperscript{2} [76]. In this model, a cross section at $E_n$ is computed as a summation of the contributions from each of $N_\lambda$ SLBW resonances [54] to the value at this energy. The value of $N_\lambda$ must be chosen, for each spin sequence, to be high enough that the addition of a nominal resonance’s contribution to the cross section values at $E_n$ is negligible. For the range of systems under investigation, an $N_\lambda$ value of 64 will produce satisfactory differential and integral results, even when applied to nuclides with relatively narrow level spacings such as $^{235}$U and $^{238}$U. This determination is based on the observations that the resulting partial reaction cross section values are unbiased at the $\sim$0.1% relative difference level when compared to values computed using a higher $N_\lambda$ value and that the $k_{\text{eff}}$ values that are computed in simulations using cross section realizations generated with 64 contributing resonances from each spin sequence are unbiased relative to the results that are obtained with additional resonances. To illustrate, the schematic in Figure 2.2 shows a realization of the $^{238}$U elastic scattering cross section localized about $E_n = 25$ keV along with the full realization. It is apparent that a truncated, local realization is sufficient to capture resonance cross section structure in the vicinity of the desired energy. Each time that a cross section value is needed within a simulation, the on-the-fly calculation method requires a new generation of an independent truncated resonance ensemble localized about $E_n$.

\textsuperscript{2}This many-level Breit-Wigner model should not be confused with the multi-level Breit-Wigner (MLBW) resonance formalism.
The SLBW elastic neutron scattering cross section is given by

\[ \sigma_n(E_n) = \sigma_{\text{pot}}(E_n) \]

\[ + \sum_{l=0}^{N_l-1} \sum_{j=1}^{N_l(l)} \sum_{\lambda=1}^{N_{\lambda}} \sigma_{\lambda} \left( \psi(\theta, x) \left[ \cos(2\phi_l(E_n)) - \left( 1 - \frac{\Gamma_{n,\lambda}}{\Gamma_{\lambda}} \right) \right] + \chi(\theta, x) \sin(2\phi_l(E_n)) \right). \]

(2.10)

The potential, or shape elastic, scattering cross section appears in the above expression and is calculated as

\[ \sigma_{\text{pot}}(E_n) = \frac{4\pi}{k^2(E_n)} \sum_{l=0}^{N_l-1} (2l + 1) \sin^2(\phi_l(E_n)). \]

(2.11)

It is well-known that, due to its neglect of level-level interference effects, the SLBW representation can result in unphysical negative elastic scattering cross sections. When a negative value is encountered on-the-fly, the elastic scattering cross section is simply set to zero. This adjustment is propagated through to the total cross section.
Radiative capture, fission, and the competitive reaction cross sections are given by

\[
\sigma_\gamma(E_n) = \sum_{l=0}^{N_l-1} \sum_{j=1}^{N_J} \sum_{\lambda=1}^{N_\lambda} \sigma_\lambda \frac{\Gamma_{\gamma,\lambda}}{\Gamma_\lambda} \psi(\theta, x),
\]

\[
\sigma_f(E_n) = \sum_{l=0}^{N_l-1} \sum_{j=1}^{N_J} \sum_{\lambda=1}^{N_\lambda} \sigma_\lambda \frac{\Gamma_{f,\lambda}}{\Gamma_\lambda} \psi(\theta, x),
\]

and

\[
\sigma_x(E_n) = \sum_{l=0}^{N_l-1} \sum_{j=1}^{N_J} \sum_{\lambda=1}^{N_\lambda} \sigma_\lambda \frac{\Gamma_{x,\lambda}}{\Gamma_\lambda} \psi(\theta, x),
\]

respectively. The total cross section is calculated as the sum of the \(N_p\) partial cross sections,

\[
\sigma_{\text{tot}}(E_n) = \sum_{i=1}^{N_p} \sigma_{r,i}(E_n),
\]

and the total resonance width, \(\Gamma_\lambda\), is calculated as the sum of the \(N_p\) partial widths,

\[
\Gamma_\lambda = \sum_{i=1}^{N_p} \Gamma_{r,i}.
\]

Other variables and formulae needed for the computation of cross sections include those for the neutron resonance energy, \(E_\lambda\); the resonance peak value,

\[
\sigma_\lambda = g_J \frac{4\pi}{k^2(E_\lambda)} \frac{\Gamma_n}{\Gamma_\lambda};
\]
the statistical spin factor,

\[ g_J = \frac{2J + 1}{4I + 2}; \tag{2.18} \]

the neutron width evaluated at the resonance energy,

\[ \Gamma_{n,\lambda}(|E_\lambda|) = \frac{\Gamma_{n,\lambda}(E_n)P_l(|E_\lambda|)}{P_l(E_n)}; \tag{2.19} \]

\[ \theta \equiv \frac{\Gamma_\lambda}{\Delta}, \tag{2.20} \]

with \( \Delta \) being the Doppler width,

\[ \Delta = 2\sqrt{k_B T E_n/A}; \tag{2.21} \]

and \( T \) being the temperature of the material in which the target nuclide resides;

\[ x \equiv \frac{2(E_n - E'_\lambda)}{\Gamma_\lambda}; \tag{2.22} \]

and the shifted resonance energy,

\[ E'_\lambda = E_\lambda + \Gamma_{n,\lambda} \frac{S_l(|E_\lambda|) - S_l(E_n)}{2P_l(|E_\lambda|)}. \tag{2.23} \]

Expressions for the penetrabilities, \( P_l \); hard-sphere phase shifts, \( \phi_l \); and resonance energy shift factors, \( S_l \), are given by
\[ P_l(\rho) = \begin{cases} 
\rho & l = 0 \\
\frac{\rho^3}{1+\rho^2} & l = 1 \\
\frac{\rho^5}{9+3\rho^2+\rho^4} & l = 2 \\
\frac{\rho^7}{225+45\rho^2+6\rho^4+\rho^6} & l = 3 \\
\frac{\rho^9}{11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8} & l = 4,
\end{cases} \quad (2.24) \]

\[ \phi_l(\rho) = \begin{cases} 
\rho & l = 0 \\
\rho - \tan^{-1}(\rho) & l = 1 \\
\rho - \tan^{-1}\left(\frac{3\rho}{3-\rho^2}\right) & l = 2 \\
\rho - \tan^{-1}\left(\frac{15\rho-\rho^3}{15-6\rho^2}\right) & l = 3 \\
\rho - \tan^{-1}\left(\frac{105\rho-10\rho^3}{105-45\rho^2+\rho^4}\right) & l = 4,
\end{cases} \quad (2.25) \]

and

\[ S_l(\rho) = \begin{cases} 
0 & l = 0 \\
-\frac{1}{1+\rho^2} & l = 1 \\
-\frac{18+3\rho^2}{9+3\rho^2+\rho^4} & l = 2 \\
-\frac{675+90\rho^2+6\rho^4}{225+45\rho^2+6\rho^4+\rho^6} & l = 3 \\
-\frac{41100+4725\rho^2+270\rho^4+10\rho^6}{11025+1575\rho^2+135\rho^4+10\rho^6+\rho^8} & l = 4,
\end{cases} \quad (2.26) \]

respectively.

Continuous-energy Doppler broadening, as opposed to the pointwise kernel broadening of the SIGMA1 method [58], is accomplished using the Voigt profile representation [77] of the symmetric and asymmetric Breit-Wigner line shape functions \( \psi \) and \( \chi \), respectively [78]. These functions are given by
\[ \psi(\theta, x) = \frac{\theta \sqrt{\pi}}{2} \text{Re} \left[ W \left( \frac{\theta x}{2}, \frac{\theta}{2} \right) \right] \]  

(2.27)

and

\[ \chi(\theta, x) = \frac{\theta \sqrt{\pi}}{2} \text{Im} \left[ W \left( \frac{\theta x}{2}, \frac{\theta}{2} \right) \right] . \]  

(2.28)

The \( W \)-function, also known as the Faddeeva function, is expressed as

\[ W(\alpha, \beta) = \exp \left( -z^2 \right) \text{erfc} \left( -iz \right) = \frac{i}{\pi} \int_{-\infty}^{\infty} dt \frac{\exp \left( -t^2 \right)}{z - t} \]  

(2.29)

with \( \alpha \) and \( \beta \) being the real and imaginary components, respectively, of complex number \( z = \alpha + i\beta \).

### 2.2.3 Additional Details

The foregoing sections provide an outline of the implementation of an on-the-fly URR cross section calculation capability. Still, however, there are numerous practical details which must be addressed in order to ensure the implementation’s robustness. The preservation of temperature correlation effects and the use of calculated cross sections within a transport code — two primary concerns — are discussed in Sections 2.2.3.1 and 2.2.3.2, respectively.

#### 2.2.3.1 Temperature Correlation

With the presented procedures for sampling resonance parameters and subsequently calculating temperature-dependent cross section values, the relationship that exists
between cross section values at different temperatures, for a given nuclide and fixed
energy, can be preserved with relative ease. When a neutron streams into a region that
contains a nuclide which was also contained in another region previously traversed
by the same neutron, without any interactions in between, the cross section values
in the two different regions must be related, regardless of temperature. A new set of
resonances should not be generated when the neutron passes into the latter region.
The same resonances should be used to compute cross sections in both regions, with
any differences due to Doppler broadening only. With the on-the-fly method, this is
accomplished by simply storing the set of resonance parameters, which is generated
for the current energy, between interactions and use it to compute cross sections at
any required temperature. Similar functionality is possible with the probability table
method [63].

2.2.3.2 Self-Shielding Factors

As another practical point of implementation, URR cross section values, once com-
puted, can be utilized in one of two ways. For a given nuclide, the evaluated nuclear
data file prescribes which of these treatments to use via the LSSF ENDF-6 flag. In the
first case, indicated by an LSSF flag set to 0, cross section values computed from File 2
unresolved resonance parameters using the above equations are to be simply added
to any background File 3 cross sections. In the second, indicated by an LSSF flag
set to 1, the computed cross section values are divided by pre-computed, averaged,
infinite-dilute values. The resulting self-shielding factors are then multiplied by the
cross section values given in File 3 to obtain the cross section values that are to be
used in the transport simulation.
2.3 Results and Analysis

One drawback of the probability table method is that data must be pre-generated at multiple energies for each desired temperature. In simulations of systems with many temperatures (e.g., high-fidelity fast reactor analyses), this can result in a large memory requirement. Calculating URR cross sections on-the-fly, directly from temperature-independent average resonance parameters, can reduce this burden significantly [79]. As an additional benefit, the need for performing the sensitivity studies that are required to ensure that probability tables are generated on a discrete phase-space mesh that is sufficiently fine is also eliminated because the on-the-fly method is continuous in the energy, temperature, and cross section magnitude variables. This feature allows the method to be used in the validation of discrete probability table data. Use of the on-the-fly method as a probability table data validation tool is presented in Section 2.3.1.

Also owing to its direct calculation of URR cross sections from nuclear data evaluation files, rather than pre-generation of probability table data, the on-the-fly method allows rapid benchmarking of URR evaluations. In addition to being a useful tool for testing the adequacy of the URR evaluations found in the major international libraries, the on-the-fly method can be used to test prospective URR evaluations during the nuclear data evaluation process itself. The ease and transparency of calculating URR cross sections directly from a trial ENDF-6 file, thus eliminating the use of an intermediate nuclear data processing code, may be of some utility to evaluators. An example of the on-the-fly method’s use as a benchmarking tool is presented in Section 2.3.2.

All simulations are performed using the ENDF71x neutron data library [80]. Where needed, probability tables are also drawn from ENDF71x. This library contains ENDF/B-VII.1 nuclear data [13] processed into ACE format with the NJOY Nuclear Data Processing System, version 99.393 [81]. Resonance parameters and other variables required for on-the-fly cross section calculations are taken from the unprocessed
ENDF/B-VII.1 ENDF-6 files.

2.3.1 Probability Table Validation

Results obtained from OpenMC simulations of a fresh fuel LWR pin cell, a model of the Big Ten critical assembly [82], and a model of the Zero Energy Breeder Reactor Assembly (ZEBRA) [83] are presented in Sections 2.3.1.1 to 2.3.1.3, respectively. Descriptions of the pin cell, Big Ten, and ZEBRA models can be found in Appendix B. Using various URR cross section treatments, multiplication factors and neutron flux spectra tallied using the ECCO-2000 energy group structure [84] are calculated for each system. Particular emphasis is placed on the comparisons of results obtained from simulations using probability tables and on-the-fly cross sections. Such comparisons can be used to validate that probability table data are generated on an $E_n-T-\sigma_t$ mesh that is sufficiently fine to reproduce results of interest.

2.3.1.1 LWR Pin Cell

The LWR fresh fuel pin cell lattice model under consideration is simulated at both hot, zero-power (HZP) and hot, full-power (HFP) conditions. In both cases all materials are at 600 K, except for the HFP case which has fuel at 900 K. URR treatments are applied to $^{234}$U, $^{235}$U, and $^{238}$U. All other nuclides are treated with averaged URR cross sections. Upon examination of the various results, it is apparent that the selection of a particular URR treatment has a negligible effect on results, as is expected for a thermal system.

Table 2.1: HZP LWR pin cell $k_{\infty}$

<table>
<thead>
<tr>
<th>URR Cross Sections</th>
<th>$k_{\infty}$</th>
<th>1(\sigma)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy-averaged</td>
<td>1.35587</td>
<td>0.00004</td>
</tr>
<tr>
<td>Probability tables</td>
<td>1.35617</td>
<td>0.00004</td>
</tr>
<tr>
<td>On-the-fly</td>
<td>1.35610</td>
<td>0.00004</td>
</tr>
</tbody>
</table>
In Tables 2.1 and 2.2, $k_{\infty}$ eigenvalue results are given for different URR cross section calculation methods. At HFP all results agree to within $1\sigma$ or $2\sigma$ for relatively tight $1\sigma$ statistical uncertainty values of 4 pcm. Very close agreement is also observed at HZP except for that modeling resonance structure in these simulations with either probability tables or on-the-fly cross sections does result in $\sim$30 pcm of positive reactivity relative to the averaged cross section case.
on-the-fly and probability table cross sections result in flux spectra that agree very well.

2.3.1.2 Big Ten

The next system to be investigated is a benchmark model of the Big Ten critical assembly. Where an on-the-fly treatment is indicated, it is applied to each nuclide in the model — $^{234}$U, $^{235}$U, $^{236}$U, and $^{238}$U. Probability tables are again taken from the ENDF71x library.

Table 2.3 gives the $k_{\text{eff}}$ results for different URR cross section treatments. Accounting

---

3IEU-MET-FAST-007, case 4 from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [85]
for the resonance structure of URR cross sections with either probability tables or on-the-fly calculations results in a \(\sim 400\) pcm increase in \(k_{\text{eff}}\) relative to the case in which averaged cross sections are utilized. Agreement to within a 1\(\sigma\) value of <10 pcm between the probability table and on-the-fly eigenvalues is observed.

Table 2.3: Big Ten \(k_{\text{eff}}\)

<table>
<thead>
<tr>
<th>URR Cross Sections</th>
<th>(k_{\text{eff}})</th>
<th>1(\sigma)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy-averaged</td>
<td>1.00085</td>
<td>0.00006</td>
</tr>
<tr>
<td>Probability tables</td>
<td>1.00466</td>
<td>0.00006</td>
</tr>
<tr>
<td>On-the-fly</td>
<td>1.00461</td>
<td>0.00006</td>
</tr>
</tbody>
</table>

Figure 2.5: Big Ten flux spectra

Good agreement is also observed between on-the-fly and probability table flux spectra and can be seen in Figure 2.5. The largest differences at energies with an appreciable flux are less than one percent. With the continuous phase-space on-the-fly method serving as the reference, agreement between on-the-fly and probability table \(k_{\text{eff}}\) values

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and flux spectra provides further validation of the discrete probability table data contained in ENDF71x.

### 2.3.1.3 ZEBRA

Finally, results of simulations of a benchmark model\(^4\) of an intermediate/fast spectrum \(k_\infty\) zone experiment conducted at the ZEBRA facility are presented. This system is selected for its extreme sensitivity to the modeling of resonance structure in the URR. On-the-fly treatments, when used, are only applied to \(^{235}\text{U}\) and \(^{238}\text{U}\) with structured URR cross sections for other nuclides coming from ENDF71x probability tables.

<table>
<thead>
<tr>
<th>Table 2.4: ZEBRA (k_\infty)</th>
</tr>
</thead>
<tbody>
<tr>
<td>URR Cross Sections</td>
</tr>
<tr>
<td>--------------------</td>
</tr>
<tr>
<td>Energy-averaged</td>
</tr>
<tr>
<td>Probability tables</td>
</tr>
<tr>
<td>On-the-fly</td>
</tr>
</tbody>
</table>

Table 2.4 highlights both the necessity of modeling URR resonance structure in simulations of ZEBRA and good agreement between the \(k_\infty\) values computed with probability tables and on-the-fly cross sections. It is important to note, however, that while accounting for structure in URR cross sections results in a \(\sim1000\) pcm reactivity increase relative to the infinite-dilute cross section case, state-of-the-art transport codes utilizing state-of-the-art processed nuclear data libraries still under-predict the experimental benchmark \(k_\infty\), 1.03000±0.00250, by more than 1000 pcm. This suggests an issue with the underlying ENDF/B-VII.1 \(^{238}\text{U}\) URR evaluation — the same evaluation adopted by all major evaluated nuclear data libraries.

Figure 2.6 shows the neutron flux computed with both the on-the-fly method and probability tables. Agreement between the two flux spectra is an indication that

\(^4\text{MIX-MET-FAST-008, core 8H from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [85]}\)
Figure 2.6: ZEBRA flux spectra

the probability tables are generated with an $E_nT\sigma_t$ mesh that is sufficiently fine to produce accurate tallies for the ECCO-2000 energy group structure that is used in these simulations.

2.3.2 Benchmarking URR Evaluations

Here, using models for ZEBRA, Big Ten, and a traveling wave reactor (TWR) unit cell (all described in Appendix B), the on-the-fly method is used to demonstrate the effect that varying the URR energy bounds can have in simulations of fast spectrum systems. Figures 2.7 to 2.9 plot the multiplication factors computed with varying URR upper energy bounds for ZEBRA, Big Ten, and the TWR unit cell, respectively.
Figure 2.7: Variation of ZEBRA $k_\infty$ with $^{238}$U upper URR energy bound

Figure 2.8: Variation of Big Ten $k_{\text{eff}}$ with $^{238}$U upper URR energy bound
Figure 2.9: Variation of TWR unit cell $k_\infty$ with $^{238}$U upper URR energy bound

The upward trend of eigenvalue with increasing upper bound suggests that resonance structure may be important at energies above the current ENDF/B-VII.1 $^{238}$U URR evaluation. As further indication of this, simulations utilizing Fröhner’s complete evaluation [86], which extends up to 300 keV, result in $k_\infty$ values that are $\sim$200 pcm closer to the ZEBRA benchmark value than those computed using the truncated ENDF/B-VII.1 evaluation. When Fröhner’s 20–300 keV evaluation is used in tandem with the URR resonance parameters tabulated at 300 keV being held constant and utilized in the 300–400 keV interval, the upward trend of $k_\infty$ persists. Increases in $k$-eigenvalues on the order of $\sim$100 pcm are also observed in analogous simulations of Big Ten and the TWR unit cell lending further credence to the supposition that the ENDF/B-VII.1 $^{238}$U URR evaluation should be extended to higher energies.

The reason for the trend becomes clear after examining Figures 2.10 and 2.11 which show the ZEBRA flux spectrum with an overlay of the $^{238}$U URR and realizations of the $^{238}$U total cross section generated for different energy bounds, respectively.
Figure 2.10: ZEBRA flux spectrum with $^{238}$U URR highlighted

Figure 2.11: $^{238}$U RRR and URR total cross sections at 293.6 K
In Figure 2.10 it is clear that the system flux peaks just above the upper energy bound of the ENDF/B-VII.1 $^{238}$U URR evaluation. It is also clear in Figure 2.11 that cross section resonance structure persists above this energy up to, and presumably beyond, 300 keV. By not accounting for the resonance structure that is present at energies above the ENDF/B-VII.1 evaluation, self-shielding effects are neglected precisely where flux peaks. The implications of this neglect are the same as those previously discussed, namely under-predicted $k$-eigenvalues. It is postulated here that utilization of an evaluation which accounts for resonance structure at energies still higher than the 300 keV bound in Fröhner’s evaluation is likely to produce a non-negligible positive reactivity effect in simulations of ZEBRA-8H — the $k_{\infty}$ of which is routinely under-predicted by $\sim$1000 pcm in simulations making use of state-of-the-art evaluated data, processed libraries, and transport codes — as well as simulations of other fast spectrum systems.

2.3.3 Computational Efficiency

With respect to runtime, the computational expense of calculating URR cross sections on-the-fly in the course of a simulation may be relatively severe, or quite manageable, relative to the probability table method, depending on the type of simulation. For example, in a basic criticality simulation of the Big Ten model, with only a $k_{\text{eff}}$ tally, the on-the-fly method is observed to run 10–20 times slower than the probability table method. However, in a simulation with more complex tallies, similar to those that may be required in practical fast reactor analysis simulations, the runtime overhead associated with the on-the-fly method is reduced to 10–20%.\cite{5} Longer runtimes can be expected when the on-the-fly method is applied to more nuclides. However, this impact will be reduced, in a relative sense, if reaction rate tallies of practical

\footnote{\textsuperscript{5}The referenced simulation consists of absorption, fission, and energy production tallies for each of four nuclides in one hundred equal-lethargy bins across a regular spatial mesh with 30 cells along each axis sized to cover the entire assembly.}
complexity are calculated in the simulation.

Because on-the-fly computations rely on temperature-independent unresolved resonance parameters rather than probability tables of arbitrary number and size, memory reduction is achieved with the method. For example, the probability tables for the four nuclides in the Big Ten model account for 71 kB per temperature while the unresolved resonance parameter data needed for on-the-fly calculations take up a total of only 16 kB, independent of the number of temperatures. For this reason, even greater memory reductions are attainable in simulations with transient or spatially-varying temperature distributions because probability table data are likely to be required at several temperatures to ensure that interpolation errors are sufficiently small, whereas the on-the-fly method allows for the calculation of cross sections continuously in temperature from a single set of unresolved resonance parameters. Also, there are URR resonance parameters given for 267 of the 423 nuclides in the ENDF/B-VII.1 evaluated data library. In systems containing more of these nuclides, further memory reductions will be realized with the on-the-fly method relative to probability tables.

2.4 Conclusions

A procedure for computing URR cross sections on-the-fly in Monte Carlo neutron transport codes without reliance on a pre-processing step, such as probability table generation, is presented. The method is used as a tool for the validation of probability table data through comparisons of both integral and differential tallies that are calculated using on-the-fly cross sections with those obtained using probability tables. This is demonstrated in simulations of intermediate/fast spectrum systems which are highly-sensitive to URR resonance structure effects. The flexibility enabled by on-the-fly cross section calculations is also shown to be exploitable in the benchmarking of URR evaluations. Used as an evaluation benchmarking tool, the on-the-fly URR cross section calculation capability reveals a phenomenon which may be
partially responsible for a longstanding discrepancy between experimental benchmark and state-of-the-art simulation results for a well-known intermediate/fast spectrum critical assembly.
Chapter 3

Probability Table Interpolation

3.1 Background

An on-the-fly scheme for calculating temperature-dependent URR cross sections directly from average resonance parameters was recently investigated [79] and detailed in Chapter 2. The most common procedure for incorporating URR cross section resonance structure into Monte Carlo neutron transport simulations, however, is the probability table method [64]. The method relies on the random sampling of tables of pre-generated cross section bands, each being characterized by its probability of being sampled, a total cross section magnitude, and partial cross section magnitudes that are conditional on the total cross section magnitude. The capability to generate these tables is implemented in many established nuclear data processing codes such as NJOY [81], PREPRO [46], AMPX [47], and CALENDF [48].

The aim of this chapter is to present a procedure for on-the-fly calculations of temperature-dependent URR cross sections through interpolation of pre-generated probability tables and examine the efficacy of this procedure. This approach involves the generation of equiprobable cross section magnitude surfaces on an energy-temperature mesh.
Within a simulation, the surfaces are sampled and interpolated in energy and temperature to obtain cross section values on-the-fly. This is in contrast to the common practices of pre-generating probability tables at all discrete temperatures present in a model, creating pseudomaterials by mixing nuclear data at two bounding temperatures [87], or statistical interpolation between temperatures [50]. It is also clearly different than the on-the-fly methodology expounded in Chapter 2.

The methods by which cross section bands are pre-generated, then sampled and interpolated within a simulation are described, as are the results of tests of the implementation of these methods, in Section 3.2. The results of further analyses of the use of these methods in Monte Carlo simulations of an integral criticality safety benchmark are presented in Section 3.3. Concluding remarks are given in Section 3.4.

3.2 Implementation

The methods used to generate and sample cross section probability tables are outlined in this section. Though the specific details of probability table generation capabilities vary by code, certain general features are common to most implementations. These commonalities are documented elsewhere [65, 66, 67, 63] and will only be outlined briefly here. Section 3.2.1 provides this outline while also emphasizing the amendments to the typical procedure which allow for the generation of equiprobable bands. The interpolation schemes that are investigated for the on-the-fly calculation of temperature-dependent cross sections are then detailed in Section 3.2.2. The results of both differential cross section and integral benchmark testing, including code-to-code comparisons with the NJOY-generated ENDF71x processed nuclear data library [80], are given in Section 3.2.3.
3.2.1 Generation of Equiprobable Cross Section Bands

Though precise cross section values in the URR are unknown, average resonance parameters can be deduced through a combined examination of the parameters of resolved resonances and fitting of gross structure in the unresolved region. These parameters are tabulated by incident neutron energy, $E_n$, and provided in ENDF-6 format [10] nuclear data evaluations. Additionally, theoretical statistical distributions of URR resonance parameters are well-known. For example, the distance in energy, $D_{l,J}$, between adjacent resonances with orbital angular momentum $l$ and total angular momentum $J$ is described by Wigner’s surmise for level spacings, introduced earlier as Equation (2.1).

Partial reaction widths, $\Gamma_{r}^{l,J}$, can be obtained by sampling a $\chi^2$-distribution, introduced earlier as Equation (2.3), with a number of degrees of freedom, $\mu_r$, that depends on the reaction, $r$. An ensemble of URR resonances can be randomly generated by sampling these resonance parameter distributions.

For a single temperature, $T$, the probability table method usually first proceeds by establishing monotonically increasing grids in both the incident neutron energy and total cross section magnitude, $\sigma_t$, variables. The $\sigma_t$ grid defines the cross section bands with band $b$ containing all $\sigma_t$ on the interval $[\sigma_t^b, \sigma_t^{b+1})$. Then, one realization of URR resonances is generated and temperature-dependent cross section values are calculated. If multiple temperatures are required, the same set of resonances is used at each temperature in order to preserve spatial and/or temporal temperature correlation effects. Though any formalism can be used, a summation over SLBW resonances is the standard prescribed by the ENDF-6 format. These formulae are the same as those given in Chapter 2.

A schematic showing an $E_n$-$\sigma_t$ mesh imposed on one realization of URR cross sections is displayed in Figure 3.1. At each energy, the index of the band containing the $\sigma_t$ magnitude is recorded, as is the value itself. The tallied values are indicated with
In addition, partial reaction cross section values that are conditional on the band of the total cross section magnitude are recorded. After many independent realizations of cross section structure are tallied, at each energy, the probability of having a total cross section in a given band is simply the number of realizations that fall within that band divided by the total number of realizations, i.e.,

\[ P(\sigma^b(E_n, T) \leq \sigma_t(E_n, T) \leq \sigma^{b+1}(E_n, T)) = \frac{|\sigma^b|}{|\sigma|} \]  

(3.1)

where \( \sigma \) and \( \sigma^b \) are the sets of all total cross section magnitude values and those total cross section magnitudes falling within band \( b \), respectively. \(|\sigma|\) and \(|\sigma^b|\) are then the cardinalities of these sets. The probabilities will generally differ both between bands
at a single energy and in a single band across energies.

The mean \( \sigma_t \) for each band can also be determined by dividing the sum of cross section magnitudes that fall within a band by the number of magnitudes within that band, or

\[
\langle \sigma_t^b(E_n, T) \rangle = \frac{\sum_{i=1}^{\lvert e^b \rvert} \sigma_{t,i}^b(E_n, T)}{\lvert \sigma_t^b \rvert}.
\] (3.2)

Mean reaction cross sections that are conditional on the band of the total cross section can be computed in an analogous manner as

\[
\langle \sigma_r^b(E_n, T) \rangle = \frac{\sum_{i=1}^{\lvert e^b \rvert} \sigma_r(E_n, T \mid \sigma_{t,i}^b(E_n, T))}{\lvert \sigma_t^b \rvert}.
\] (3.3)

In order to capture the effects of URR resonance structure, transport codes can then sample a probability-\( \sigma_t \) pair — simultaneously obtaining partial cross sections conditional on the sampled \( \sigma_t \) — each time that new cross section values are needed in a simulation.

The implementation utilized in this work results in the generation of probability bands which are each equiprobable across all energies and temperatures bounded by the selected \( E_n-T \) grid. That is, the probability of sampling band \( b \) is the same for all \( E_n-T \) pairs on the grid. This is accomplished by, first, storing all realizations of total and conditional partial cross section values at a single \( E_n-T \) pair and ordering those realizations by \( \sigma_t \) magnitude. Then the \( \sigma_t \) grid values are adjusted such that each probability band has some specific, desired probability. Holding these target band probabilities constant as this process is repeated at each \( E_n-T \) pair ensures the generation of equiprobable bands over the entire \( E_n-T \) grid. In the case of equal
target probabilities for all bands, forcing $|\sigma^b|$ to be constant yields the desired band probabilities and, with this constraint, Equations (3.2) and (3.3) can be used to compute band total and conditional partial reaction cross sections, respectively. An illustration of these equiprobable bands, which can be visualized as surfaces on an $E_n$-$T$ grid, is found in Figure 3.2 which shows 8 surfaces, each with a 0.125 probability of being sampled.

![Figure 3.2: Equiprobable $^{238}$U total cross section surfaces](image)

### 3.2.2 On-the-Fly Temperature Interpolation

One typical treatment of probability table data in Monte Carlo codes requires that tables be generated at each discrete temperature that is present in the model of the system being simulated. For models with highly-detailed temperature distributions, this results in a massive increase in probability table data and computer memory...
requirements. In order to mitigate this problem, an on-the-fly method for calculating temperature-dependent cross section values directly from resonance parameters at each event within a simulation is investigated in Chapter 2. This approach is very memory efficient because it relies only on temperature-independent average resonance parameters. With respect to simulation runtime for simple criticality calculations, though, it can be quite inefficient\(^1\) due to the sampling of resonance parameters and calculation of cross sections at each event. Taken together, the increased memory requirements associated with using a fine probability table temperature grid and the calculational inefficiency of the on-the-fly method point to the need for an interpolation scheme which allows for the fast calculation of URR cross sections at all intermediate points on a coarse temperature grid.

The generation and interpolation of equiprobable cross section surfaces on an \(E_n-\sigma_t\) grid is one possible solution. In this work, these surfaces are pre-generated as described in the previous section and then utilized in the continuous-energy Monte Carlo neutron transport code OpenMC [68]. Each time that new URR cross section values are needed within a simulation, an equiprobable band, which contains both \(\sigma_t\) and conditional partial cross sections, is sampled. This automatically fixes the four points on the \(E_n\)-\(T\) grid that must be interpolated between.

Once a band is sampled, cross section values are interpolated between bounding energies at each bounding temperature. The two new energy-interpolated values are then interpolated in temperature. The interpolation scheme to be used for the \(E_n\) variable is set in the ENDF-6 file for a given nuclide. A summary of allowed schemes for interpolation between lower and upper bounding energies — \(E_L\) and \(E_H\), respectively — to a desired energy, \(E_n\), is given in Table 3.1. Specification of the scheme for interpolation between lower and upper bounding temperatures — \(T_L\) and \(T_H\), respectively — to a desired temperature, \(T\), is left to the user and may be selected from any one of those given in Table 3.2. These are the same five interpolation

\(^1\)In high-fidelity fast reactor analysis simulations the runtime penalty will not be as severe due to other overhead associated with detailed tallies, communication between multiphysics packages, etc.
schemes that were previously used in an investigation of cross section temperature interpolation in the resolved resonance region [88].

Table 3.1: Summary of energy interpolation schemes

<table>
<thead>
<tr>
<th>Descriptor</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma(E_n, T)$ (constant)</td>
<td>$\sigma(E_n, T) = \sigma(E_L, T)$</td>
</tr>
<tr>
<td>$E_n \cdot \sigma(E_n, T)$ (linear-linear)</td>
<td>$\sigma(E_n, T) = \sigma(E_L, T) + \frac{E-E_n}{E_H-E_L} \left[ \sigma(E_H, T) - \sigma(E_L, T) \right]$</td>
</tr>
<tr>
<td>$E_n \cdot \ln [\sigma(E_n, T)]$ (linear-log)</td>
<td>$\sigma(E_n, T) = \sigma(E_L, T) \exp \left( \frac{E-E_n}{E_H-E_L} \ln \left[ \frac{\sigma(E_H, T)}{\sigma(E_L, T)} \right] \right)$</td>
</tr>
<tr>
<td>$\ln [E_n] - \sigma(E_n, T)$ (log-linear)</td>
<td>$\sigma(E_n, T) = \sigma(E_L, T) + \frac{\ln [E/E_L]}{\ln [E_H/E_L]} \left[ \sigma(E_H, T) - \sigma(E_L, T) \right]$</td>
</tr>
<tr>
<td>$\ln [E_n] - \ln [\sigma(E_n, T)]$ (log-log)</td>
<td>$\sigma(E_n, T) = \sigma(E_L, T) \exp \left( \frac{\ln [E/E_L]}{\ln [E_H/E_L]} \ln \left[ \frac{\sigma(E_H, T)}{\sigma(E_L, T)} \right] \right)$</td>
</tr>
</tbody>
</table>

3.2.3 Numerical Code Verification

In order to test the implementation of the probability table generation capability, code-to-code comparisons with NJOY are performed. First, the SLBW calculation routines are used to reconstruct pointwise, continuous-energy cross sections from ENDF/B-VII.1 nuclear data [13]. These values are compared to those computed with NJOY99.393 for the ENDF71x processed nuclear data library. Elastic scattering cross sections computed with both codes, using the same set of resonance parameters, are shown in Figures 3.3 and 3.4. The relative difference between the pointwise values is seen to be within the commonlyaccepted target tolerance of 0.1%.

Then, the routines which sample resonance parameters and tally the calculated URR cross section magnitudes are tested in a comparison of the infinite-dilute values computed with the new implementation and NJOY2012.50. The $^{238}$U infinite-dilute elastic scattering cross sections are shown in Figure 3.5. With a target 1σ statistical uncertainty of 0.1%, close agreement is observed between the values calculated with each code.
Table 3.2: Summary of temperature interpolation schemes

<table>
<thead>
<tr>
<th>Descriptor</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T$-$\sigma(E_n, T)$ (linear-linear)</td>
<td>$\sigma(E_n, T) = \sigma(E_n, T_L) + \frac{T-T_L}{T_H-T_L} [\sigma(E_n, T_H) - \sigma(E_n, T_L)]$</td>
</tr>
<tr>
<td>$T$-$\ln[\sigma(E_n, T)]$ (linear-log)</td>
<td>$\sigma(E_n, T) = \sigma(E_n, T_L) \exp \left( \frac{T-T_L}{T_H-T_L} \ln \left[ \frac{\sigma(E_n, T_H)}{\sigma(E_n, T_L)} \right] \right)$</td>
</tr>
<tr>
<td>$\sqrt{T}$-$\sigma(E_n, T)$ (sqrt-linear)</td>
<td>$\sigma(E_n, T) = \sigma(E_n, T_L) + \frac{\sqrt{T}-\sqrt{T_L}}{\sqrt{T_H}-\sqrt{T_L}} [\sigma(E_n, T_H) - \sigma(E_n, T_L)]$</td>
</tr>
<tr>
<td>$\sqrt{T}$-$\ln[\sigma(E_n, T)]$ (sqrt-log)</td>
<td>$\sigma(E_n, T) = \sigma(E_n, T_L) \exp \left( \frac{\ln \left[ \frac{T}{T_L} \right]}{\ln \left[ \frac{T_H}{T_L} \right]} \ln \left[ \frac{\sigma(E_n, T_H)}{\sigma(E_n, T_L)} \right] \right)$</td>
</tr>
<tr>
<td>$\ln[T]$-$\ln[\sigma(E_n, T)]$ (log-log)</td>
<td>$\sigma(E_n, T) = \sigma(E_n, T_L) \exp \left( \frac{\ln \left[ \frac{T}{T_L} \right]}{\ln \left[ \frac{T_H}{T_L} \right]} \ln \left[ \frac{\sigma(E_n, T_H)}{\sigma(E_n, T_L)} \right] \right)$</td>
</tr>
</tbody>
</table>

Figure 3.3: $^{239}$U elastic scattering cross sections, 293.6 K
Figure 3.4: $^{243}$Pu elastic scattering cross sections, 293.6 K

Figure 3.5: $^{238}$U infinite-dilute elastic scattering cross sections
Integral testing of the new probability table capability is performed using the Big Ten critical assembly benchmark model which is described in Appendix B. The results of room temperature $k_{\text{eff}}$ calculations are given in Table 3.3. Excellent agreement is observed between eigenvalues computed using the probability tables generated with NJOY99.393 and the new implementation.

### Table 3.3: Code-to-code comparison of Big Ten $k_{\text{eff}}$

<table>
<thead>
<tr>
<th>Probability Tables</th>
<th>$k_{\text{eff}}$</th>
<th>1σ</th>
</tr>
</thead>
<tbody>
<tr>
<td>ENDF71x (NJOY99.393)</td>
<td>1.00464</td>
<td>0.00005</td>
</tr>
<tr>
<td>New Implementation</td>
<td>1.00456</td>
<td>0.00004</td>
</tr>
</tbody>
</table>

### 3.3 Results and Analysis

With the satisfactory performance of the probability table generation capability demonstrated in the results of the testing described in Section 3.2.3, it is now appropriate to investigate the extent to which the $E_n$-$T$-$\sigma_t$ mesh used for interpolation to intermediate energies and temperatures is able to reproduce results obtained with cross section data that are generated exactly at the intermediate variable values or on a very fine mesh. Both differential cross section values and integral multiplication factor results computed with OpenMC are presented in Sections 3.3.1 and 3.3.2, respectively.

#### 3.3.1 Differential Cross Sections

In order to determine how fine of a phase-space mesh is required to reproduce reference differential cross section values, temperature and energy grid refinement studies are presented in Sections 3.3.1.1 and 3.3.1.2, respectively. These studies compare temperature-dependent and energy-dependent cross section magnitude values for a
single band that are generated by interpolation with different $E_n$ and $T$ discretizations to fine-mesh reference values.

### 3.3.1.1 Temperature Grid Interpolation

Figures 3.6 to 3.10 show the greatest $^{238}\text{U}$ total cross section magnitude band with different numbers of temperature intervals spanning 293.6–2500 K. All cross section values are for a single energy (20 keV) and number of magnitude bands (16). This energy is chosen because it is the lower URR energy bound for $^{238}\text{U}$ where resonance structure is more pronounced relative to higher URR energies. The number of bands is selected because, as is later shown, it is sufficiently large to capture resonance self-shielding effects in cases of interest. It can be seen that only 17 temperature grid points are required to reproduce the fine-mesh cross section values to $\sim 1.0\%$.

![Figure 3.6: $^{238}\text{U}$ band 16 total cross section with 1 temperature interval at 20 keV](image)

Figure 3.6: $^{238}\text{U}$ band 16 total cross section with 1 temperature interval at 20 keV
Figure 3.7: $^{238}$U band 16 total cross section with 2 temperature intervals at 20 keV

Figure 3.8: $^{238}$U band 16 total cross section with 4 temperature intervals at 20 keV
Figure 3.9: $^{238}$U band 16 total cross section with 8 temperature intervals at 20 keV

Figure 3.10: $^{238}$U band 16 total cross section with 16 temperature intervals at 20 keV
To ensure that 17 temperature grid points is also sufficient to closely reproduce reference cross section values for other magnitude bands, plots of the lowest and eight-lowest bands are shown in Figures 3.11 and 3.12, respectively. With 17 grid points, the interpolated temperature-dependent cross section values at 20 keV differ from the fine-mesh values by less than 0.5%.

Figure 3.11: $^{238}$U band 1 total cross section with 16 temperature intervals at 20 keV

### 3.3.1.2 Energy Grid Interpolation

Figures 3.13 to 3.17 show the greatest $^{238}$U total cross section magnitude band with different numbers of energy grid points. All cross section values are for a single temperature (293.6 K) and number of magnitude bands (16). This temperature is chosen because resonance structure is more pronounced at lower temperatures. The number of bands is again selected due to being sufficient to capture resonance self-
shielding effects, as will be demonstrated. With only 32 energy points spanning the entire $^{238}\text{U}$ URR, fine-mesh cross section values are reproduced to $\sim 1.0\%$.

Now, to check that interpolation between 32 energy grid points reproduces reference cross section values for other magnitude bands, plots of bands 1 and 8 are generated and shown in Figures 3.18 and 3.19, respectively. With 32 grid points the interpolated energy-dependent cross section values at 293.6 K typically differ from the fine-mesh values by less than 0.5%.
Figure 3.13: $^{238}$U band 16 total cross section with 2 energies at 293.6 K

Figure 3.14: $^{238}$U band 16 total cross section with 4 energies at 293.6 K
Figure 3.15: $^{238}$U band 16 total cross section with 8 energies at 293.6 K

Figure 3.16: $^{238}$U band 16 total cross section with 16 energies at 293.6 K
Figure 3.17: $^{238}$U band 16 total cross section with 32 energies at 293.6 K

Figure 3.18: $^{238}$U band 1 total cross section with 32 energies at 293.6 K
3.3.2 Integral Benchmarks

With differential cross section band values calculated via interpolation agreeing with fine-mesh reference values to within commonly-accepted margins, integral results are now compared. In these comparisons the $k_{\text{eff}}$ for Big Ten is computed at 100 K intervals from 350 K to 2350 K using both temperature interpolation and the on-the-fly treatment presented in Chapter 2. The on-the-fly results are taken to be reference solutions because they are continuous in $E_n$, $T$, and $\sigma_t$. Convergence of the phase-space mesh is then determined using the root-mean-square (RMS) difference in $k_{\text{eff}}$ values, RMS $\Delta k_{\text{eff}}$. Temperature, energy, and cross section magnitude band refinement studies are described in Sections 3.3.2.1 to 3.3.2.3, respectively.
3.3.2.1 Temperature Grid Refinement

RMS $\Delta k_{\text{eff}}$ values computed with each temperature interpolation scheme and different numbers of temperature intervals are plotted in Figure 3.20. With each interpolation scheme, 16 temperature intervals gives a negligibly lower RMS $\Delta k_{\text{eff}}$ than 8 intervals indicating a sufficiently refined temperature grid. For a fixed number of temperature points, though, $\ln (T) - \ln (\sigma_t)$ temperature interpolation typically better reproduces the on-the-fly reference result.

Comparisons of the results obtained with explicit interpolation on equiprobable $E_n$-$T$ surfaces with other methods that are currently used in production codes are also conducted. Statistical temperature interpolation, which is employed by MC21, utilizes probability table data generated at discrete temperatures. When data at an
intermediate temperature is required in a simulation, the data at one of the discrete, bounding temperatures is selected based on the linear proximity of the intermediate temperature to each bound. That is, the data at $T_L$ is selected with probability

$$p(T_L) = 1 - \frac{T - T_L}{T_H - T_L}$$

and the data at $T_H$ is selected with a probability of $1 - p(T_L)$. The RMS $\Delta k_{\text{eff}}$ values computed with both explicit and statistical interpolation are plotted in Figure 3.21 as a function of the number of temperature intervals. While, for a fixed number of intervals, explicit $\ln(T)\ln(\sigma_t)$ temperature interpolation typically performs better than statistical interpolation, the performance of the two methods is practically identical.
with 16 intervals.

Another approach for treating the temperature dependence of nuclear data is to select data generated at the greatest temperature which is still lower than the target intermediate temperature. Such an approach is employed by MCATK [89] for treating resolved resonance region cross section data. The RMS $\Delta k_{\text{eff}}$ values computed with both this lower-neighbor method and $\ln(T)-\ln(\sigma_t)$ temperature interpolation are plotted in Figure 3.22. As in the case of statistical interpolation, the lower-neighbor treatment produces results which are comparable with explicit interpolation using just 16 intervals, though explicit interpolation typically results in a lower RMS $\Delta k_{\text{eff}}$ for lower fixed numbers of intervals.
3.3.2.2 Energy Grid Refinement

Figure 3.23: Big Ten RMS $\Delta k_{\text{eff}}$ with $\ln T - \ln \sigma_t$ temperature interpolation, 16 bands

The RMS $\Delta k_{\text{eff}}$ values computed with a varying number of discrete energy grid points are plotted in Figure 3.23. Explicit $\ln T - \ln \sigma_t$ temperature interpolation along with 16 cross section magnitude bands are utilized in each case. A grid consisting of 32 energy points appears to be sufficiently fine to reproduce the on-the-fly reference results.

3.3.2.3 Band Grid Refinement

The RMS $\Delta k_{\text{eff}}$ values for Big Ten that are computed with a varying number of discrete cross section magnitude bands are plotted in Figure 3.24. Each case makes use of explicit $\ln T - \ln \sigma_t$ temperature interpolation and 32 energies. Using 16 equiprobable
3.4 Conclusions

A method for generating equiprobable cross section magnitude bands is presented and the explicit interpolation of those bands in temperature within continuous-energy Monte Carlo neutron transport simulations is demonstrated. In code-to-code testing, differential cross sections and integral benchmark tallies computed with the new implementation show good agreement with reference solutions. In simulations requiring temperature interpolation, cross sections computed with each of the investigated interpolation schemes are shown to reproduce reference $k_{\text{eff}}$ eigenvalues relatively well.
over a broad range of temperatures relevant to reactor analysis with just 16 interpolation intervals. This interpolation makes use of data which consumes ~100 kB of computer memory per nuclide. Consequently, the interpolation of temperature-dependent probability bands appears to be a promising candidate method for the treatment of URR cross sections in the presence of spatial and/or temporal temperature variations.
Chapter 4

Multi-Level and Competitive Reaction Resonance Effects

4.1 Background

As is required by the ENDF-6 format [10], the probability table method [64], which is used by many production-level continuous-energy Monte Carlo particle transport codes for modeling cross section resonance structure in the URR, is typically implemented using the SLBW resonance formalism to generate cross sections.\footnote{One exception is CALENDF [48] which allows SLBW, multi-niveau Breit-Wigner (MNBW), and Reich-Moore formalisms.}

Here, effects of the use of the multi-level Breit-Wigner (MLBW) resonance formalism, as specified by the ENDF-6 format, for on-the-fly URR cross section reconstruction are investigated. The implementation and testing of an MLBW cross section calculation capability are presented in Section 4.2 along with the results and analyses of simulations which compare single-level and multi-level treatments of URR resonance structure.
Also required by the ENDF-6 format is the treatment of so-called competitive reaction cross sections as infinite-dilute in the URR. More precisely, reactions other than elastic scattering, capture, and fission are modeled as having the smooth, pointwise cross sections found in File 3 of an ENDF-6 file. As a consequence, level inelastic scattering cross sections are commonly modeled as being energy-averaged in Monte Carlo transport codes. However, resonance structure in the cross sections of these reactions does, in fact, exist in nature.

While results obtained in calculations with the TRIPOLI Monte Carlo transport code [5], which makes use of nuclear data processed with CALENDF [48], have hinted at the significance of modeling competitive reaction resonance structure using the average competitive reaction partial width provided with URR evaluations in File 2 of ENDF-6 files [90, 91], the effects of rigorously modeling this resonance structure have largely gone unexamined. Section 4.3 contains further explorations of the phenomenon of URR competitive reaction cross section resonance structure, an implementation for modeling it in transport simulations, and results obtained from simulations in which it is modeled.

Lastly, conclusions with respect to both multi-level and competitive reaction cross section resonance structure effects are given in Section 4.4.

4.2 Multi-Level Resonance Formalisms

It is well-known that, due to its neglect of level-level interference effects, the SLBW resonance formalism can produce unphysical negative cross section values in the troughs which occur just below resonance energies where interference between resonance scattering and potential scattering reaction components is most pronounced [10]. Even at energies where SLBW cross sections do not turn negative, there can be significant differences with cross sections computed with an MLBW formalism. To illus-
trate, Figure 4.1 shows both SLBW and MLBW reconstructions of the ENDF/B-VII.1 $^{238}$U elastic scattering cross section in the URR at a temperature of 0.1 K. The modifications to the SLBW cross section calculation procedure that must be made when switching to the MLBW formalism are discussed in Section 4.2.1. Verification of this MLBW calculation procedure is given in Section 4.2.1.1

In principle, the most faithful representation of experimentally observed cross section data in transport calculations will follow from using the same formalism to reconstruct cross sections from parameters as was used to derive those parameters in the evaluation process. These analyses differ from previous examinations of alternate resonance formalisms for the treatment of URR cross sections which looked primarily at using multi-level fits to URR data in the evaluation process in order to back out average resonance parameters [92]. In this work, parameters are taken, as is, and used to reconstruct cross sections with the different formalisms. The aim here is to determine, for a fixed set of resonance parameters, whether or not level-level interference effects impact tally results of interest. Conclusions based on these relative results are not invalidated by the inconsistency that arises when two different formalisms are used in the data evaluation and data processing procedures, but rather, can be applied in analyses of the impact of that inconsistency.

Results computed using multi-level URR cross sections computed on-the-fly are compared to those obtained using the standard on-the-fly SLBW model in simulations of intermediate/fast spectrum systems in Section 4.2.2. Comparisons of results obtained by using the same stochastically-generated realization of resonance parameters in both the SLBW and MLBW formalisms, which allow for the quantification of level-level interference effects on integral tallies such as $k_{eff}$ and energy group reaction rates, are also presented.
4.2.1 Implementation of the ENDF-6 MLBW Formalism

In the ENDF-6 format version of the MLBW formalism, only elastic scattering cross sections are reconstructed using multi-level equations. The single-level equations are used to reconstruct the cross sections for all other reactions. In order to allow on-the-fly Doppler broadening with the $\psi$-$\chi$ Doppler integrals, the MLBW elastic scattering cross section is coded as...
\[
\sigma_n(E_n) = \frac{4\pi}{k^2(E_n)} \sum_{l=0}^{N_l-1} (2l + 1) \sin^2(\phi_l(E_n)) + \sum_{l=0}^{N_l-1} \sum_{j=1}^{N_J(l)} \sum_{\lambda=1}^{N_\lambda} \sigma_\lambda \\
\times \left( \psi(\theta, x) \left[ \cos(2\phi_l(E_n)) - \left( 1 - \frac{\Gamma_{n,\lambda}}{\Gamma_{\lambda}} \right) \right] + \frac{G_{l,\lambda}}{\Gamma_{n,\lambda}} \right) \\
+ \chi(\theta, x) \left[ \sin(2\phi_l(E_n)) + \frac{H_{l,\lambda}}{\Gamma_{n,\lambda}} \right]
\]

where \( G_{l,\lambda} \) is defined as

\[
G_{l,\lambda} \equiv \frac{1}{2} \sum_{j'=1}^{N_J(l)} \sum_{\lambda'=1; j'=j}^{N_\lambda} \frac{\Gamma_{n,\lambda} \Gamma_{n,\lambda'}}{(E_\lambda - E_{\lambda'})^2 + (\Gamma_\lambda + \Gamma_{\lambda'})^2/4} \] (4.2)

and \( H_{l,\lambda} \) is defined as

\[
H_{l,\lambda} \equiv \sum_{j'=1}^{N_J(l)} \sum_{\lambda'=1; j'=j}^{N_\lambda} \frac{E_\lambda - E_{\lambda'}}{(E_\lambda - E_{\lambda'})^2 + (\Gamma_\lambda + \Gamma_{\lambda'})^2/4}. \] (4.3)

While the mechanics of sampling resonance parameters are unchanged relative to the SLBW case, the computational cost of calculating cross section values is increased significantly when using the MLBW equations due to the double summation over resonances that is required in computing the \( G_{l,\lambda} \) and \( H_{l,\lambda} \) factors.

### 4.2.1.1 Numerical Code Verification

In order to test the implementation of the MLBW cross section capability, code-to-code comparisons with NJOY are performed. The MLBW calculation routines are used to reconstruct pointwise, continuous-energy cross sections from ENDF/B-VII.1
nuclear data [13]. These values are compared to those computed with NJOY99.393 for the ENDF71x processed nuclear data library. Elastic scattering cross sections computed with both codes, using the same set of resonance parameters, are shown in Figures 4.2 and 4.3. The relative differences between the pointwise values are seen to be within the commonly-accepted target tolerance of 0.1% at virtually all energies.

4.2.2 Results and Analysis

The MLBW URR cross section calculation capability implemented in OpenMC is used in simulations of four systems. HZP and HFP LWR pin cell lattice results are presented in Section 4.2.2.1. Models of the intermediate/fast spectrum Big Ten and
ZEBRA critical assemblies are used to obtain the results shown in Sections 4.2.2.2 and 4.2.2.3, respectively. Descriptions of the pin cell, Big Ten, and ZEBRA models can be found in Appendix B. For each model, multiplication factors and neutron flux spectra tallied using the ECCO-2000 energy group structure are presented. Elastic scattering rate spectra are computed for both the Big Ten and ZEBRA models using the ECCO-33 energy group structure.

4.2.2.1 LWR Pin Cell

First, a pressurized-water reactor pin cell model is simulated at HZP conditions with the UO$_2$ fuel, clad, and moderator all at 600 K. The $k_\infty$ eigenvalue computed with the on-the-fly SLBW cross sections is given in Table 4.1 along with the value computed
with an MLBW treatment. At a $1\sigma$ uncertainty value of $\sim5$ pcm the SLBW and MLBW results are statistically indistinguishable. Similar agreement between $k_{\infty}$ eigenvalues obtained in simulations of the same pin cell model, only at HFP conditions (i.e., 900 K fuel), can be seen in Table 4.2.

The SLBW and MLBW flux spectra computed for both the HZP and HFP models are compared in Figures 4.4 and 4.5, respectively. As in the case of the integral $k_{\infty}$ tallies, the SLBW and MLBW flux spectra exhibit very close agreement. This agreement between SLBW and MLBW results for both pin cell models is not all that surprising as it has been demonstrated that the effects of representing URR cross section resonance structure are of negligible consequence in simulations of thermal power reactor systems. So, if neglecting URR resonance structure entirely does not impact simulation results it is reasonable to suppose that the formalism used when structure is modeled matters quite little.
Figure 4.4: HZP LWR pin cell flux spectra

Figure 4.5: HFP LWR pin cell flux spectra
4.2.2.2 Big Ten

Table 4.3: Big Ten $k_{\text{eff}}$

<table>
<thead>
<tr>
<th>URR Cross Sections</th>
<th>$k_{\text{eff}}$</th>
<th>1σ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy-averaged</td>
<td>1.00085</td>
<td>0.00006</td>
</tr>
<tr>
<td>On-the-fly SLBW</td>
<td>1.00461</td>
<td>0.00006</td>
</tr>
<tr>
<td>On-the-fly MLBW</td>
<td>1.00462</td>
<td>0.00006</td>
</tr>
</tbody>
</table>

Turning to a system which is known to be sensitive to the modeling of URR cross section resonance structure, it is again observed that the $k_{\text{eff}}$ values computed using on-the-fly SLBW cross sections and on-the-fly MLBW cross sections are in extremely close agreement. These values can be seen in Table 4.3. This close agreement suggests that the use of a multi-level resonance formalism may not be necessary to reproduce many integral tallies of interest.

Figure 4.6: Big Ten flux spectra
This suggestion is further supported by the agreement between the flux spectra and $^{238}\text{U}$ elastic scattering rate spectra, which are shown for both formalisms, in Figures 4.6 and 4.7, respectively.

### 4.2.2.3 ZEBRA

<table>
<thead>
<tr>
<th>URR Cross Sections</th>
<th>$k_{\text{eff}}$</th>
<th>$1\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy-averaged</td>
<td>1.00910</td>
<td>0.00005</td>
</tr>
<tr>
<td>On-the-fly SLBW</td>
<td>1.01913</td>
<td>0.00006</td>
</tr>
<tr>
<td>On-the-fly MLBW</td>
<td>1.01918</td>
<td>0.00005</td>
</tr>
</tbody>
</table>

Looking at another system which is known to be highly-sensitive to the modeling of URR cross section resonance structure, it is observed that the ZEBRA $k_{\infty}$ values
computed using on-the-fly SLBW cross sections and on-the-fly MLBW cross sections, displayed in Table 4.4, are in extremely close agreement, just as they are for Big Ten. The ZEBRA SLBW and MLBW $k_\infty$ values are statistically indistinguishable at a $1\sigma$ uncertainty of $<10$ pcm.

![ZEBRA flux spectra](image)

Figure 4.8: ZEBRA flux spectra

Close agreement between differential tallies is also observed in the ZEBRA simulations. The flux spectra and $^{238}$U elastic scattering rate spectra — computed with both on-the-fly SLBW cross sections and on-the-fly MLBW cross sections — are plotted in Figures 4.8 and 4.9, respectively.

Table 4.5: ZEBRA $k_\infty$

<table>
<thead>
<tr>
<th>URR Cross Sections</th>
<th>$k_{\text{eff}}$</th>
<th>$1\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single SLBW realization</td>
<td>1.01851</td>
<td>0.00005</td>
</tr>
<tr>
<td>Single MLBW realization</td>
<td>1.01859</td>
<td>0.00006</td>
</tr>
</tbody>
</table>
Figure 4.9: ZEBRA $^{238}$U elastic scattering rate spectra

Noting that the calculation of on-the-fly cross sections with either formalism relies on the generation of a new set of resonances at each event, the possible effects of level-level interference in simulations using the same set of resonance parameters throughout a simulation are now investigated. That is, the same, single realization of resonance parameters is used throughout an entire simulation, once with the equations of the SLBW formalism and once with those of the MLBW formalism. These simulations allow one to gauge the extent to which differences between SLBW and MLBW simulations are artificially averaged out when a new resonance structure is generated at each event. Table 4.5 shows the $k_\infty$ eigenvalues that are computed when using the same set of resonance parameters in each of the formalisms. Again, extremely close agreement is observed between the SLBW and MLBW results which are statistically indistinguishable at a 1σ uncertainty of <10 pcm.
The flux spectra and $^{238}$U elastic scattering rate spectra are also tallied in these simulations. These results are plotted in Figures 4.10 and 4.11, respectively. It can be seen that, while the differences between SLBW and MLBW tallies at the energies corresponding to the URR of $^{238}$U are somewhat greater than in the event-based resonance structure generation cases, they are typically well below 1% and do not exhibit any clear bias (i.e., the relative differences between the SLBW and MLBW results fluctuate rapidly between being positive or negative at any given energy).

Though all presented results indicate that multiplication factor and flux spectra tallies are largely insensitive to the choice of URR resonance formalism, one can envision cases where significant differences in calculated results would arise. One example is a shielding problem with a monoenergetic source at a URR energy where SLBW and MLBW cross sections differ appreciably. These differences would have a strong, direct
effect on the penetration of neutrons into a material.

### 4.3 Competitive Reaction Resonance Structure

Correctly accounting for the URR resonance structure in cross sections for reactions other than elastic scattering, capture, and fission in transport simulations is complicated not so much by the physics in question — the cross section resonance structure of a reaction for which resonance parameters exist should, quite obviously, be modeled — but by the three-way coupling of the representation of resonance parameters and cross sections according to ENDF-6 format standards, codes used to process that evaluated data, and transport codes that utilize the processed data.
The ENDF-6 format allows the specification of File 2 unresolved resonance parameters for only elastic scattering, capture, fission, and a single, additional competitive reaction — typically inelastic scattering to the first excited level of the compound nucleus, if energetically possible. Any resonance structure in another reaction is to be described entirely via pointwise energy-cross section pairs in File 3.\(^2\)

![Figure 4.12: \(^{238}\text{U} \) level inelastic scattering cross sections](image)

Further, despite allowing for the specification of URR resonance parameters for a competitive reaction, the ENDF-6 format prescribes the use of only the smoothed, pointwise File 3 cross section values for that reaction. These energy-averaged File 3 cross sections will generally, at a specific energy, differ significantly from the values that are produced when competitive reaction partial widths are sampled and used to reconstruct cross sections using the equations of a resonance formalism. This can be

\(^2\)Any structure that is represented in the File 3 background cross section is typically quite crude because it is only the gross structure over multiple URR resonances, not the structure of individual resonances.
seen in Figure 4.12 which shows the File 3 $^{238}$U level inelastic scattering cross section along with a realization of the cross section reconstructed from sampled resonance parameters.

The possibility of different treatments of the competitive reaction cross section inducing biases in simulation results is mentioned in an earlier code-to-code comparison [90, 91]. In that study of Big Ten critical assembly simulations, it is noted that the TRIPOLI code [5], in making use of URR cross section data generated with the CALENDF nuclear data processing code [48], accounts for resonance structure in the competitive reaction cross section. Many other transport codes, such as MCNP [93], utilize the infinite-dilute URR cross section values that are produced by the NJOY Nuclear Data Processing System [81]. Here, in OpenMC, competitive reaction cross section resonance structure effects are isolated by allowing for the on-the-fly use of either averaged or structured values in the same code. The implementation of this capability is discussed briefly in Section 4.3.1 and results obtained in simulations utilizing it are provided in Section 4.3.2.

### 4.3.1 Implementation of Competitive Resonance Structure

The key difference between implementing the capability to model the resonance structure of a competitive reaction and any other reaction is the determination of whether the use of competitive partial widths to reconstruct a partial reaction cross section is allowable. For the elastic scattering, capture, and fission reactions, if an average partial width is present at any incident neutron energy of interest, it may be used to sample a $\chi^2$ distribution for partial widths to generate a realization of resonance parameters. The mere presence of an average competitive width at a given energy, however, does not guarantee the validity of using the value to generate a realization of parameters. Many nuclides’ URR evaluations cover energy intervals over which multiple competitive reactions’ channels are open. As a consequence, a single competitive reaction width may be provided over an energy range in which multiple
competitive reactions are possible. Determining the effect of a single partial competitive width on the resonance structure of multiple underlying reaction cross sections is not straightforward. Therefore, it is only appropriate to use a nuclide’s average partial competitive width for generating a realization of partial widths if there is a single open competitive reaction. Where the competitive reaction partial width is taken into account in this work, it is applied only at the energies at which a single reaction besides elastic scattering, capture, and fission is possible, thus eliminating ambiguity. If this criterion is met, a realization of partial widths may be generated and calculating the competitive reaction’s resonance cross section is as simple as using Equation (2.14). The verification of the partial width sampling and cross section calculation routines presented earlier are applicable here, as well.

### 4.3.2 Results and Analysis

The capability to model the URR resonance structure of competitive reaction cross sections is used in simulations of the same four systems as in Section 4.2.2 — an LWR pin cell at HZP and HFP conditions, Big Ten, and ZEBRA. The results of these simulations are presented in Sections 4.3.2.1 to 4.3.2.3, respectively.

For each model, $k$ eigenvalues and neutron flux spectra tallied using the ECCO-2000 energy group structure are computed with different combinations of URR cross section calculation methodology and competitive reaction cross section representation. Each simulation employs one of three combinations: File 3 pointwise, infinite-dilute URR cross sections with no modeling of competitive reaction resonance structure (except to the extent that any structure appears in the File 3 cross sections); structured SLBW URR cross sections computed on-the-fly for only elastic scattering, capture, and fission; and structured SLBW URR cross sections computed on-the-fly for elastic scattering, capture, fission, and a single competitive reaction for selected nuclides.
4.3.2.1 LWR Pin Cell

Table 4.6: HZP LWR pin cell $k_\infty$

<table>
<thead>
<tr>
<th>URR Cross Sections</th>
<th>Competitive Cross Section</th>
<th>$k_\infty$</th>
<th>1σ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy-averaged</td>
<td>Energy-averaged</td>
<td>1.35587</td>
<td>0.00004</td>
</tr>
<tr>
<td>On-the-fly</td>
<td>Energy-averaged</td>
<td>1.35610</td>
<td>0.00004</td>
</tr>
<tr>
<td>On-the-fly</td>
<td>Resonance structure</td>
<td>1.35618</td>
<td>0.00004</td>
</tr>
</tbody>
</table>

Table 4.7: HFP LWR pin cell $k_\infty$

<table>
<thead>
<tr>
<th>URR Cross Sections</th>
<th>Competitive Cross Section</th>
<th>$k_\infty$</th>
<th>1σ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy-averaged</td>
<td>Energy-averaged</td>
<td>1.34574</td>
<td>0.00004</td>
</tr>
<tr>
<td>On-the-fly</td>
<td>Energy-averaged</td>
<td>1.34581</td>
<td>0.00004</td>
</tr>
<tr>
<td>On-the-fly</td>
<td>Resonance structure</td>
<td>1.34579</td>
<td>0.00004</td>
</tr>
</tbody>
</table>

In Tables 4.6 and 4.7, $k_\infty$ eigenvalue results at both HZP and HFP conditions, respectively, do not differ outside of a relatively tight $2\sigma$ statistical uncertainty of $\sim10$ pcm whether $^{238}$U first-level inelastic scattering cross section resonance structure is modeled or not.\(^3\)

The flux spectra plots in Figures 4.13 and 4.14 show negligible differences at both HZP and HFP conditions, respectively, depending on whether or not the $^{238}$U competitive reaction resonance structure is modeled. This agreement between $k_\infty$ eigenvalues and flux spectra is expected for the same reason that SLBW and MLBW calculations produce similar results: in general, modeling the resonance structure of any URR cross sections does not have a significant impact in simulations of thermal power reactor systems.

\(^3\)A competitive partial width is not provided for $^{234}$U or $^{235}$U in the ENDF/B-VII.1 evaluation.
Figure 4.13: HZP LWR pin cell flux spectra

Figure 4.14: HFP LWR pin cell flux spectra
4.3.2.2 Big Ten

Table 4.8: Big Ten $k_{\text{eff}}$

<table>
<thead>
<tr>
<th>URR Cross Sections</th>
<th>Competitive Cross Section</th>
<th>$k_{\text{eff}}$</th>
<th>$1\sigma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy-averaged</td>
<td>Energy-averaged</td>
<td>1.00085</td>
<td>0.00006</td>
</tr>
<tr>
<td>On-the-fly</td>
<td>Energy-averaged</td>
<td>1.00461</td>
<td>0.00006</td>
</tr>
<tr>
<td>On-the-fly</td>
<td>Resonance structure</td>
<td>1.00530</td>
<td>0.00006</td>
</tr>
</tbody>
</table>

Table 4.8 gives the $k_{\text{eff}}$ results for different URR cross section treatments. As was shown in Table 2.3, accounting for the resonance structure of URR cross sections with on-the-fly calculations results in a $\sim 375$ pcm increase in $k_{\text{eff}}$ relative to the case in which averaged cross sections are utilized. Modeling the resonance structure of the $^{238}\text{U}$ first-level inelastic scattering reaction cross section contributes another $\sim 70$ pcm of positive reactivity.
The flux spectra computed both with and without inelastic scattering cross section resonance structure modeled are plotted in Figure 4.15. When inelastic scattering cross section resonance structure is introduced into the URR treatment, a 2–4% decrease in flux is seen across a relatively wide energy interval at the lower end of the spectrum due to the reduced inelastic scattering rate in the URR relative to the averaged cross section case. This is precipitated by a 2–4% increase in flux within the $^{238}$U URR which is also due to the reduced inelastic scattering rate. In other words, less URR inelastic scattering in the structured cross section case means that neutrons are transferred less frequently from the URR to lower energies. This translates to increases and decreases in flux within the URR and below it, respectively.

4.3.2.3 ZEBRA

<table>
<thead>
<tr>
<th>URR Cross Sections</th>
<th>Competitive Cross Section</th>
<th>$k_\infty$</th>
<th>1σ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy-averaged</td>
<td>Energy-averaged</td>
<td>1.00910</td>
<td>0.00005</td>
</tr>
<tr>
<td>On-the-fly</td>
<td>Energy-averaged</td>
<td>1.01913</td>
<td>0.00006</td>
</tr>
<tr>
<td>On-the-fly</td>
<td>Resonance structure</td>
<td>1.02057</td>
<td>0.00005</td>
</tr>
</tbody>
</table>

Table 4.9 contains the $k_\infty$ results for the different URR cross section treatments. As was shown in Table 2.4, accounting for the resonance structure of URR cross sections with on-the-fly calculations results in a $\sim$1000 pcm increase in $k_\infty$ relative to the case in which averaged cross sections are utilized. Modeling the resonance structure of the $^{238}$U first-level inelastic scattering reaction cross section contributes another $\sim$150 pcm of positive reactivity.

The flux spectra computed both with competitive reaction cross section resonance structure modeled and with energy-averaged pointwise competitive reaction cross sections are plotted in Figure 4.16. When inelastic scattering cross section resonance structure is introduced into the URR treatment, a decrease in flux of 2–4% is seen over a wide interval at lower energies for the same reason as in the Big Ten simulations:
Figure 4.16: ZEBRA flux spectra

A reduced inelastic scattering rate in the URR relative to the averaged cross section case. Similarly, a 2–4% increase in flux within the URR of $^{238}$U is observed.

### 4.4 Conclusions

A capability to calculate URR cross sections on-the-fly with the ENDF-6 version of the MLBW formalism is implemented in a continuous-energy Monte Carlo code. Code-to-code comparisons with NJOY99.393 are performed and show close agreement between both codes’ computed pointwise MLBW resonance cross sections. The new capability is used in analyses of the effects of modeling URR resonance structure with a multi-level formalism. Very close agreement between the $k$ eigenvalues, and flux and reaction rate spectra, computed with SLBW and MLBW cross sections suggests...
that the use of a multi-level formalism may not be required in computing URR cross sections for many applications of interest. Extension of the implementation beyond the ENDF-6 version of MLBW by accounting for level-level interference effects in the cross sections for reactions other than elastic scattering should be considered.

Also implemented is a capability to model the cross section resonance structure of a single competitive reaction in the URR. Accounting for this structure, as opposed to using an energy-averaged cross section representation, results in $\sim 70$ pcm and $\sim 150$ pcm of positive reactivity in simulations of Big Ten and ZEBRA, respectively. If average URR partial widths are provided for multiple competitive reactions (rather than a single one) in future nuclear data evaluations, it may be of interest to model the resonance structure for each of those reactions.
Chapter 5

Independent Resonance
Realizations by Simulation

5.1 Background

While Chapter 4 focuses on physical models and assumptions that are typically used in the process of actually calculating a single URR cross section, this chapter explores the implications of the root cause of the URR phenomenon, which is to say a lack of knowledge of resonance structure down to the level of individual resonances. This is a fundamentally different type of uncertainty than is usually discussed when dealing with resolved resonances. To be sure, there are uncertainties in resolved resonance data which can impact simulation results. However, the uncertainties on resolved resonance parameters propagate to uncertainties on cross section values, not the underlying resonance structure. Thought of another way, resolved resonance parameters are deterministic and result in energy-dependent cross section values with some uncertainty — typically no more than a few percent for the principal reactions of the nuclides which are most relevant to nuclear science and technology applications. Contrast this with the stochastic nature of the URR in which the energy and partial
widths of any single resonance are entirely unknown and must be randomly sampled from theoretical distributions.

To mitigate the problem of unknown URR resonance structure, the probability table method \cite{64} and direct, on-the-fly cross section calculations \cite{79} effectively generate a new realization of resonances at each event.\footnote{The on-the-fly approach explicitly generates a new realization at each event while the probability table method does so implicitly by sampling cross section magnitudes which represent different realizations.} This is unphysical. For all currently practical purposes, resonance parameters are constant physical properties of a neutron-nucleus system.

A natural alternative to probabilistic re-generation of URR resonance structure within a simulation is to generate a single realization of resonance parameters at the start of a simulation and use that same, unchanging realization throughout. Such a realization is still probabilistic in the sense that it is generated by sampling resonance parameters from distributions, but once sampled, a single set of resonance parameters is valid in all cross section calculations, for all neutron histories, as is the case in nature. In fact, similar solutions were briefly explored for modeling the resonance structure of URR cross sections prior to the advent, and subsequent widespread adoption, of the probability table method \cite{94, 95}. However, the methods employed to actually generate resonance realizations often made very crude approximations \cite{95, 96}. Use of the resulting fine structure cross sections in Monte Carlo calculations was generally intractable from a computational perspective. Due to the great expense of both generating resonance realizations and utilizing the continuous-energy cross section values from those realizations in any meaningful calculation, these alternate methods were largely abandoned in favor of probability table treatments. Motivated by the notion that a single, persistent URR realization is, in many ways, a better model of nature and enabled by modern computational resources, it is appropriate to revisit single URR resonance ensemble realizations for use in Monte Carlo simulations.

With such a treatment, though, the question looms: how does one know that the single
realization generated accurately represents the true resonance structure which exists in nature? The answer, of course, is that one cannot ever make that determination. In fact, the sampled resonance structure will invariably be a poor representation of nature, at least with respect to cross section values at specific energies. Though a sampled resonance ensemble will constitute a viable realization of nature because it is reconstructed from a set of resonance parameters that is drawn from a distribution of physically allowable values, no single realization can be trusted more or less than any other realization to represent the single, true cross section resonance structure which exists in nature. It would take an infinite number of realizations to stumble upon this real ensemble, and one could not even recognize it if he did because the resonance parameters which describe the actual URR resonances are, by definition, unknown. For this reason, some efforts were aimed at developing methods for generating a recommended realization [97] and also quantifying integral calculation uncertainties that arise from a lack of knowledge of the true URR resonance structure [94, 98]. These efforts, too, were largely abandoned with the adoption of probability table methods.

One possible solution to the above dilemma is to generate independent realizations of URR resonance structure and utilize each of these realizations throughout its own independent Monte Carlo transport simulation. By doing so, expected value tallies which are more rigorous than those obtained from simulations relying on probability tables are accessible. Also, with each independent simulation now representing a viable realization of nature, it is possible to determine the statistical spread of tally results. This spread represents the uncertainty induced by a lack of knowledge of URR resonance structure and cannot be ascertained using the probability table or on-the-fly methods. The ability to compute more rigorous expected values and the loss of that ability when using probability tables are discussed further in Section 5.2. The implementation of the capability to generate independent resonance ensembles and utilize them within a transport simulation are sketched out it Section 5.3. Results of simulations performed with the continuous-energy Monte Carlo neutron transport
code OpenMC which demonstrate the calculation of expected values and corresponding uncertainties are presented in Section 5.4. A summarizing discussion is found in Section 5.5.

### 5.2 Independent Realizations Versus Probability Table Sampling

The typical probability table algorithm [64] and the newly-introduced on-the-fly method [79] both assume that neutrons, at a given energy, experience resonance structure that is independent of all structure previously encountered. The result is an artificial averaging over all possible resonance structures whereas, in nature, a single resonance structure exists. As a consequence, it is not guaranteed that simulations using probability tables or on-the-fly calculations must reproduce true expected value tallies. In general, the re-generation of a new resonance structure at each event will introduce a bias in calculated results.

In other words, the value obtained by taking the mean of the tally results of \( N \) independent simulations, each using cross sections from one of \( N \) independent URR resonance structure realizations throughout, gives the expected value for the tally. On the other hand, taking the mean of the tally results of \( N \) independent simulations, each using probability tables, gives a value that is based on \( N \) simulations which each utilize cross sections representing several different realizations of resonance structure at once. This difference between results computed with probability tables and those computed by averaging independent simulations can be illustrated with a simple example:

If there is a point-source at \( E_0 \),
\[ S(E) = S_0 \int_{-\infty}^{\infty} dE \delta(E - E_0), \] (5.1)

and there are exactly two equiprobable resonance structures,

\[ \Sigma_1(E_0 \rightarrow E_1) = 0; \]
\[ \Sigma_1(E_1 \rightarrow E_2) = \infty; \] (5.2)
\[ \Sigma_1(E_2) = 0 \]

and

\[ \Sigma_2(E_0 \rightarrow E_1) = \infty; \]
\[ \Sigma_2(E_1) = 0; \] (5.3)
\[ \Sigma_2(E_2) = 0, \]

one concludes that two independent simulations, each utilizing a different one of the two possible realizations, yield an expectation of 0.5 interactions for each of the \( S_0 \) source particles, whereas probability tables yield 0.75. The probabilities of the possible outcomes are summarized in Table 5.1.

<table>
<thead>
<tr>
<th>Method</th>
<th>Interactions</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>0</td>
</tr>
<tr>
<td>Probability tables</td>
<td>0.5</td>
</tr>
<tr>
<td>Independent realizations</td>
<td>0.5</td>
</tr>
</tbody>
</table>

While this admittedly contrived example illustrates the presence of a bias resulting from the generation of an entirely new resonance structure at each event, in practice,
the magnitude of such a bias is often quite acceptable, even imperceptible, as is shown in Section 5.4.

5.3 Implementation of Single URR Realizations

The implementation of the capability to generate a single realization of URR resonance parameters for continued use throughout a simulation requires only straightforward modifications to the on-the-fly capability presented in Chapter 2. The mechanics of sampling level spacings and partial reaction widths are unchanged. At the initialization of a simulation, before any neutron histories are run, starting from the highest-energy resolved resonance region resonance with a given spin sequence, the Wigner distribution for level spacings, Equation (2.1), is sampled to determine the distance in energy to the next resonance with that same spin sequence. Using this new resonance energy as a starting point, another level spacing is sampled to determine the placement of the next, and so on. For each resonance energy that is sampled, partial neutron, capture, fission, and competitive widths are also sampled using Equation (2.3), thus completing the specification of the corresponding resonance. The process is terminated once several resonances above the upper URR energy bound have been generated. Extension of the realization beyond the upper bound is needed so that cross sections calculated at an energy just below the bound have the appropriate contribution from resonances existing at both higher and lower energies. The result of neglecting resonances above the upper URR energy bound would be diminished cross section magnitudes just below the crossover to the fast energy region. A similar extension of the resonance generating procedure to energies below the lower URR energy bound is not required as the resolved resonance parameters themselves can be used — albeit in a resonance formalism (SLBW) that may be different than the one in which they are represented in File 2 — to calculate a contribution to cross section values at the lower end of the URR.
Once a complete realization of resonances — specified by their resonance parameters — is generated over the required energy range for each spin sequence, it can be utilized in a simulation. Procedures presented in Chapter 2 can be extended easily enough to accomplish this as well. Instead of an on-the-fly generation of an energy-localized realization of resonance parameters and on-the-fly cross section calculation using those parameters, as was described in Chapter 2, the same realization of resonance parameters generated at the initialization of a simulation is utilized in all cross section calculations throughout a simulation. Whenever a nuclide’s cross sections must be calculated within a simulation, a number of resonances about the current neutron energy are identified and their parameters are used to compute the contributions of each of those resonances to the partial cross section values at the desired energy. In this process, if a nuclide’s cross sections are calculated at a specific energy, identical cross section values will be computed in subsequent calculations at that same energy (cf. [64, 79]). As a corollary, cross section values computed at energies which neighbor one another will reflect the correlated resonance structure between the two energies. That is, if cross section values are computed at a resonance energy once, all cross sections computed very close to that energy will have a similarly large magnitude. This can be important in fine mesh energy spectrum calculations which require the same resonance structure to be experienced by all neutrons at all events in order to reveal the peaks and valleys in reaction rate tallies which occur across energy as a result of individual resonances.

Generating new, independent resonance structure realizations for independent transport simulations is as simple as changing the pseudo-random number generator seed used when generating one set of resonances to a different value. Examples of independent realizations of URR resonance structure generated from the same resonance parameter distributions are shown in Figure 5.1. Because the same underlying algorithms and implementations used to generate realizations of URR resonance structure and compute cross section values in previous chapters are merely being repurposed, the numerical code verification undertaken in Section 3.2.3 applies here, as well.
5.4 Results and Analysis

The capability to utilize independent realizations of URR resonance structure is used in simulations of four systems. An LWR pin cell is simulated at HZP conditions and the results are presented in Section 5.4.1. Results of simulations of a model of the well-known fast spectrum, high-enriched uranium metal sphere Godiva are given in Section 5.4.2. Finally, models of Big Ten and ZEBRA are used to obtain the results shown in Sections 5.4.3 and 5.4.4, respectively. A description of each model can be found in Appendix B.

For each model, 250 independent transport simulations, each using a unique realization of URR resonance structure throughout, are conducted. The expected value $k$ eigenvalue tallies obtained from each batch of simulations, as well as the statisti-
cal spread of those tallies, are examined and compared to the values that one obtains using on-the-fly calculations. Additionally, each of the four distributions of 250 eigenvalue realizations is tested for normality with both the Shapiro-Wilk [99] and Anderson-Darling [100] tests. The results of these statistical tests are shown in Tables 5.2 and 5.3, respectively. The $p$-value computed in a Shapiro-Wilk test has the interpretation of being the significance value, $\alpha$, at which the null hypothesis of the normality of the sample data can be rejected. The $A^2$ statistic computed in an Anderson-Darling test has the interpretation of being the critical value above which the null hypothesis of the normality of the sample data can be rejected at the $\alpha$ corresponding to the critical value. For all distributions, at an $\alpha$ value of 5%, the null hypothesis that the eigenvalue realizations are drawn from a normal distribution cannot be rejected using either test for normality.

It is worth noting, though, that the apparent normality of the distributions is not required in order to demonstrate the two principal results which follow: a single simulation with on-the-fly cross section calculations reproduces very well the expected value obtained from multiple independent simulations and the range of eigenvalues arising from independent URR realizations can be significant. Normality of the distributions is, however, a feature which is helpful when interpreting $1\sigma$ uncertainties, standard deviations, Gaussian curve fits, etc. To that end, the distribution of eigenvalue realizations for each model is plotted and overlaid with two different Gaussian distributions. One of the distributions is simply a curve fit to the observed data using the sample expected eigenvalue, $\langle k \rangle$, and the sample standard deviation of $k$ realizations, $\text{SD}_k$. The second distribution is the Gaussian that is expected based on statistical uncertainty alone. It is also constructed using $\langle k \rangle$, but uses the sample expected value of the standard error of the mean (i.e., the mean of the 250 $1\sigma$ values), $\langle 1\sigma_k \rangle$, as its standard deviation. Comparing these two curves enables one to observe the extent to which URR resonance structure uncertainty results in a dispersion of $k$ realizations.
Table 5.2: Shapiro-Wilk normality test results

<table>
<thead>
<tr>
<th>Model</th>
<th>p-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>LWR pin cell</td>
<td>0.637</td>
</tr>
<tr>
<td>Godiva</td>
<td>0.065</td>
</tr>
<tr>
<td>Big Ten</td>
<td>0.347</td>
</tr>
<tr>
<td>ZEBRA</td>
<td>0.331</td>
</tr>
</tbody>
</table>

Table 5.3: Anderson-Darling normality test results

<table>
<thead>
<tr>
<th>Model</th>
<th>$A^2$ (5% Critical Value: 0.775)</th>
</tr>
</thead>
<tbody>
<tr>
<td>LWR pin cell</td>
<td>0.392</td>
</tr>
<tr>
<td>Godiva</td>
<td>0.694</td>
</tr>
<tr>
<td>Big Ten</td>
<td>0.440</td>
</tr>
<tr>
<td>ZEBRA</td>
<td>0.435</td>
</tr>
</tbody>
</table>

5.4.1 LWR Pin Cell

Table 5.4: HZP LWR pin cell results summary

<table>
<thead>
<tr>
<th></th>
<th>$\langle k_{\infty} \rangle$ (1σ)</th>
<th>$\langle 1\sigma_{k_{\infty}} \rangle$ (1σ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample $\langle k_{\infty} \rangle$ (1σ)</td>
<td>1.35610 (0.00003)</td>
<td></td>
</tr>
<tr>
<td>Sample SD$<em>{k</em>{\infty}}$</td>
<td>0.00044</td>
<td></td>
</tr>
<tr>
<td>Sample $\langle 1\sigma_{k_{\infty}} \rangle$ (1σ)</td>
<td>0.00041 (&lt;0.00001)</td>
<td></td>
</tr>
<tr>
<td>On-the-fly $k_{\infty}$ (1σ)</td>
<td>1.35618 (0.00004)</td>
<td></td>
</tr>
</tbody>
</table>

First, a pressurized-water reactor pin cell is modeled at HZP conditions with the UO$_2$ fuel, clad, and moderator all at 600 K. The distribution of $k_{\infty}$ eigenvalues computed from 250 independent realizations of URR resonance structure is shown in Figure 5.2 and a summary of the results is given in Table 5.4. Figure 5.2 demonstrates that the observed distribution of $k_{\infty}$ realizations is nearly identical to the distribution that is expected as a result of statistical uncertainty alone. This visual agreement is confirmed by the close agreement between the observed sample standard deviation, 0.00044, and the expected sample standard deviation, 0.00041. Table 5.4 also shows very close agreement between the actual expected eigenvalue, $\langle k_{\infty} \rangle$, which is computed by taking the mean of the 250 $k_{\infty}$ realizations, and the $k_{\infty}$ value computed with a single on-the-fly calculation in which new URR resonance structure realizations are generated at each event. Taken together, the preceding observations lead to the
somewhat expected conclusion that running multiple simulations of an LWR pin cell with different URR realizations does not provide much information that could not be obtained in a single on-the-fly simulation.

### 5.4.2 Godiva

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample (\langle k_{\text{eff}} \rangle (1\sigma))</td>
<td>0.99982 (0.00001)</td>
<td></td>
</tr>
<tr>
<td>Sample SD(k_{\text{eff}})</td>
<td>0.00012</td>
<td></td>
</tr>
<tr>
<td>Sample (\langle 1\sigma_{k_{\text{eff}}} \rangle (1\sigma))</td>
<td>0.00010 (&lt;0.00001)</td>
<td></td>
</tr>
<tr>
<td>On-the-fly (k_{\text{eff}} (1\sigma))</td>
<td>0.99969 (0.00010)</td>
<td></td>
</tr>
</tbody>
</table>

Next, a Godiva benchmark model is simulated with 250 independent simulations, each using a different URR resonance structure. The distribution of \(k_{\text{eff}}\) eigenvalues
is displayed in Figure 5.3 and a summary of the results is provided in Table 5.5. Much as in the case of the LWR pin cell, Figure 5.3 illustrates that the actual distribution of $k_{\text{eff}}$ realizations is quite similar to the distribution that is expected if only statistical uncertainty is considered. The observed sample standard deviation, 0.00012, is relatively close to the expected sample standard deviation, 0.00010. Close agreement is also seen when comparing $\langle k_{\text{eff}} \rangle$ and the single on-the-fly $k_{\text{eff}}$ value. Again, averaging multiple independent simulations having different URR realizations produces similar results as an on-the-fly simulation, as is expected considering the peak of Godiva’s exceedingly hard spectrum occurs far above the upper energy bounds of the uranium nuclides’ unresolved regions.
5.4.3 Big Ten

Big Ten is also simulated 250 times with a different URR resonance structure used in each run. The distribution of $k_{\text{eff}}$ eigenvalues is plotted in Figure 5.4 and a summary of the results is found in Table 5.6. In contrast to what is observed in the distributions of LWR pin cell and Godiva eigenvalues, Figure 5.4 shows that the realized distribution of Big Ten $k_{\text{eff}}$ values is discernibly broader than the distribution that is generated based on statistical uncertainty alone. The real, observed sample standard deviation is more than five times the expected sample standard deviation. With a Gaussian fit to the $k_{\text{eff}}$ sample, this leads to an increase in the 95% confidence interval about $\langle k_{\text{eff}} \rangle$ of more than 150 pcm. It may then be concluded that this discrepancy in standard deviations is attributable to unknown URR resonance structure. However, despite these discrepant uncertainties, close agreement between $\langle k_{\text{eff}} \rangle$ and the
| Sample $\langle k_{\text{eff}} \rangle$ (1σ) | 1.00533 (0.00003) |
| Sample SD $k_{\text{eff}}$ | 0.00055 |
| Sample $\langle 1\sigma k_{\text{eff}} \rangle$ (1σ) | 0.00010 (<0.00001) |
| On-the-fly $k_{\text{eff}}$ (1σ) | 1.00530 (0.00006) |

A single on-the-fly $k_{\text{eff}}$ value is observed. So, an on-the-fly simulation and the average of multiple independent simulations having different URR realizations yield comparable eigenvalues, but the uncertainty due to unknown URR resonance structure only reveals itself through multiple independent realizations.

### 5.4.4 ZEBRA

![ZEBRA $k_\infty$ PDF](image)

Figure 5.5: ZEBRA $k_\infty$ PDF

Finally, 250 independent simulations of ZEBRA, each utilizing a different URR res-
Table 5.7: ZEBRA results summary

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample $\langle k_\infty \rangle$ (1$\sigma$)</td>
<td>1.02077 (0.00006)</td>
<td></td>
</tr>
<tr>
<td>Sample $\text{SD}<em>{k</em>\infty}$</td>
<td>0.00096</td>
<td></td>
</tr>
<tr>
<td>Sample $\langle 1\sigma_{k_\infty} \rangle$ (1$\sigma$)</td>
<td>0.00012 (&lt;0.00001)</td>
<td></td>
</tr>
<tr>
<td>On-the-fly $k_\infty$ (1$\sigma$)</td>
<td>1.02057 (0.00005)</td>
<td></td>
</tr>
</tbody>
</table>

onance structure, are performed. The distribution of $k_\infty$ eigenvalues and a summary of the results are shown in Figure 5.5 and Table 5.7, respectively. The distribution of $k_\infty$ highlights the uncertainty in individual eigenvalue realizations due to variability in URR resonance realizations, much as in the case of Big Ten — only to a greater extent. That is, the distribution of $k_\infty$ values that are actually calculated in simulations relying on different realizations of a single URR resonance structure is much broader than the distribution which arises solely from statistical uncertainty. The observed sample standard deviation is eight times the expected sample standard deviation leading to an increase in the 95% confidence interval about $\langle k_\infty \rangle$ of more than 300 pcm, assuming a Gaussian fit to the distribution. What is more, because this additional uncertainty is based on the fundamental lack of knowledge of precise URR resonance structure, it cannot be reduced by simply simulating more neutron histories, nor can it be extracted from a simulation making use of probability tables or on-the-fly cross section calculations.

5.5 Conclusions

A capability to construct single, independent URR realizations for use throughout independent continuous-energy Monte Carlo neutron transport simulations is presented. From resonance parameters sampled at the initialization of a simulation, cross sections are calculated on-the-fly. Using this capability, which eliminates the unphysical re-generation of resonance parameters within a simulation, expected value tallies which capture the effect of a persistent URR resonance structure are calculated from multiple independent simulations of models of an LWR pin cell, Godiva,
Big Ten, and ZEBRA. Though not a theoretical requirement, these expected values tend to be in good agreement with results calculated with an on-the-fly treatment. However, \textit{the spread of eigenvalue realizations coming from simulations using independent URR realizations is much larger than that which is expected based on statistical uncertainty alone. This increased uncertainty is due to the uncertainty in the structure of URR resonances and cannot be decreased by simulating more histories.} In simulations of the intermediate/fast spectrum ZEBRA critical assembly, the 95\% confidence interval about the expected $k_\infty$ value, obtained by averaging over 250 independent simulations, is 375 pcm, more than 300 pcm of which is due to a lack of known URR resonance parameters. Ultimately, this motivates an extension of the most important nuclides’ (e.g., $^{238}$U) resolved resonance region evaluations to higher energies. Additional work should be aimed at applying this capability in simulations of more realistic fast reactor models. Along with this, the effect of URR uncertainties on other parameters of interest, such as Doppler reactivity coefficients, should be investigated.
Chapter 6

Secondary Distribution Doppler Broadening

6.1 Background

In the course of a Monte Carlo particle transport simulation, the interactions between individual particles and the materials those particles traverse must be modeled as they occur. This requires the existence of probability distributions describing the possible positions in phase-space of any outgoing particle, possibly as a function of the relative position in phase-space of the interacting particles at the start of the interaction. When modeling a neutron-nucleus interaction in a neutron transport simulation, for example, quantities such as the outgoing energy and direction of any neutron surviving or produced in the interaction are needed. The probability distributions which are sampled to obtain these values are commonly referred to as secondary distributions.

Secondary distribution data can be provided in a nuclear data evaluation in a variety of forms, depending on the nuclide and reaction, and are then translated by a nu-
clear data processing code into a form that can be utilized in a transport simulation. Common secondary distribution representations include tabular data, coefficients for Legendre polynomial expansions or other functional forms, and even resonance parameters — all at 0 K. These data are often energy-dependent which gives rise to Doppler effects if the thermal motion of target nuclei is accounted for. However, it is common practice among major nuclear data processing codes and Monte Carlo transport codes to neglect target motion when generating and sampling secondary distributions. Further, because target motion is neglected in the treatment of secondary distributions, it is also neglected in the Doppler broadening of higher-energy cross sections. In NJOY2012, the default behavior is to not perform cross section Doppler broadening above an energy equal to the minimum of 1.0 MeV, the energy of the lowest reaction threshold, and the upper bound of the RRR. This energy is usually $\sim$100 keV, depending on the nuclide. In explaining this rationale, the manual states [45]:

Caution: for use in transport codes, it is recommended to use the program default. We don’t know how to compute the spectrum of scattered neutrons from a broadened inelastic level in the current generation of codes. Broadened cross sections for threshold reactions may be useful for other purposes.

and also that:

cross sections for high velocities are normally smooth with respect to $32k_B T/A$ for any temperatures outside of stellar photospheres; therefore, they do not show significant Doppler effects.

In other words, it is recommended to ignore cross section Doppler broadening for all reactions above $\sim$100 keV because methods for calculating the secondary neutron distributions for level inelastic scattering do not exist and this is a reasonable approximation because Doppler effects are typically not important at those energies, except
at astrophysical temperatures.

The following sections are concerned with the modeling and analysis of the effects of the 0 K cross section and 0 K secondary distribution approximations for elastic scattering. The theoretical outline of a consistent treatment of the thermal motion of target nuclei when computing temperature-dependent cross sections and secondary distributions is presented in Section 6.2. The implementation of an algorithm adhering to that outline in a continuous-energy Monte Carlo code is described in Section 6.3. That implementation is then used in simulations aimed at determining the effects of correctly accounting for the temperature dependence of secondary distributions. The results of these simulations and their analyses are given in Section 6.4. Conclusions and opportunities for future work are found in Section 6.5.

6.2 Temperature-Dependent Elastic Scattering Kernels

Nuclei in a material at non-zero temperature, $T$, are in thermal motion. This motion creates a relative velocity between the neutron and target, $\vec{v}_{rel} = \vec{v}_n - \vec{v}_t$. Because distribution functions (e.g., cross sections, secondary angle/energy distributions) often exhibit dependence on energy and transport codes typically require distribution functions in terms of neutron energy, not the relative neutron-target energy value, an averaging of the distribution functions over all possible relative velocities resulting from non-zero nuclear velocities is required. The resulting averaged values are said to be *Doppler broadened*. An overview of cross section Doppler broadening is given in Section 6.2.1, maintaining consistency between temperature-dependent cross sections and ideal gas scattering kinematics is discussed in Section 6.2.2, and preserving that consistency in the sampling of secondary distributions is the topic of Section 6.2.3.
6.2.1 Doppler Broadened Cross Sections

In the context of cross sections, Doppler broadening methods are typically formulated to rigorously preserve the integrated reaction rate for reaction \( x \) by averaging the 0 K reaction cross section over all possible relative neutron-target velocities. With variations in notation, this usually appears as

\[
v_n\sigma_x(T, v_n) = \int_{v_t} \text{d}v_t V(T, v_t) v_{\text{rel}}\sigma_x(0, v_{\text{rel}})
\]

where \( V(T, v_t) \) is the probability distribution for the target velocity vector, \( \vec{v}_t \), which is often factorized into independent distributions for the cosine between the pre-collision neutron and target velocities, \( \mu_{\text{in}} \), and the target speed, \( |\vec{v}_t| \). An ideal gas model, which assumes isotropic particle direction and a Maxwell-Boltzmann distribution of energies,

\[
M(T, v_t) = \frac{4}{\sqrt{\pi}} \beta^3 v_t^2 e^{-\beta^2 v_t^2},
\]

\[
\beta \equiv \sqrt{\frac{Am_n}{2k_BT}},
\]

where \( A \) is the mass of the nucleus in units of neutron mass, \( m_n \), is usually employed for this purpose. The effective, temperature-dependent cross section, \( \sigma_x(T, v_n) \), can then be used in a transport simulation.

0 K and Doppler broadened cross sections are compared in Figures 6.1 and 6.2 which show the \(^{56}\text{Fe} \) elastic and inelastic scattering cross sections, respectively. It can be seen that accounting for the effect of thermal target motion has a definite impact on effective, temperature-dependent cross section values.
Figure 6.1: $^{56}$Fe elastic scattering cross sections

Figure 6.2: $^{56}$Fe inelastic scattering cross sections
At elevated temperatures, this is the case even in the fast energy region where Doppler broadening is usually neglected. The first step in a consistent Doppler broadening methodology is to account for the thermal motion of target nuclei at all energies when computing effective, temperature-dependent cross sections.

### 6.2.2 Ideal Gas Scattering

However, this is not enough. In the course of a Monte Carlo simulation, quantities describing the individual reaction events that occur must be known. This means that $\vec{v}_t$ and $\mu_{in}$ values must be determined at each elastic scattering event in order to correctly account for the effects of thermal target motion on the kinematics of a reaction. It is well-known that such effects lead to distortions of elastic scattering kernels at thermal energies [101] and in the vicinity of cross section resonances [102]. Historically, algorithms for sampling $\vec{v}_t$ and $\mu_{in}$ relied on an ideal gas model with an elastic scattering cross section assumed to be constant over the interval of attainable relative energies [103, 104]. More recently, sampling algorithms which eliminated the need for a constant cross section approximation via a particle weight correction [105] or a rejection sampling of the 0 K elastic scattering cross section [106] were demonstrated. When employed in state-of-the-art Monte Carlo transport codes, ideal gas scattering models relying on the constant cross section approximation cease to sample target velocities at energies above $400k_B T$ [93, 3]. Energy-dependent cross section models are typically employed at energies up to $\sim 1$ keV, still well below the energies at which cross sections are commonly Doppler broadened. The second step in a consistent Doppler broadening methodology is to model neutron-nucleus scattering kinematics with $\vec{v}_t$ and $\mu_{in}$ values sampled from a probability distribution which accounts for both the distribution of target velocities in a material and any energy-dependent structure in the elastic scattering cross section. Consistency requires that this be done at all energies.
where cross sections are Doppler broadened.

6.2.3 Doppler Broadened Secondary Distributions

In order to fully-describe an elastic scattering event, a value for the scattering cosine between the incident and outgoing neutron velocities, $\mu_{\text{out}}$, is needed. This value is sampled from the secondary distribution for the scattering nuclide. Generally, these distributions are energy-dependent which means they are susceptible to Doppler effects. This energy dependence is illustrated by the ENDF/B-VII.1 $^{56}\text{Fe}$ elastic scattering angular distribution displayed in Figure 6.3. Examination of this distribution reveals that the probability of sampling a given scattering cosine varies with energy, but does so over relatively large energy intervals ($\sim0.1\ \text{MeV}$). This can be contrasted with the secondary distribution generated from a CIELO evaluation [107], shown in
Figure 6.4, which exhibits a structure that is much more rapidly-varying in energy. The ENDF/B-VII.1 distributions are smoothed across energies and show broader structure as a result. The CIELO distributions are generated directly from resonance parameters and therefore show distortions across individual resonance energies. It is worth noting that the ACE format data bloats to $\sim 100$ MB when the detailed CIELO distributions are included.

Despite the readily-apparent energy dependence of the scattering cosine secondary distributions, it is common practice to sample these 0 K distributions at the incident neutron energy, independent of thermal target motion, with the implicit assumption being that distributions do not have significant energy dependence. **The final step in a consistent Doppler broadening methodology is to sample secondary distributions at the relative neutron-nucleus energy corresponding to the**
\( \vec{v}_t \) and \( \mu_{\text{in}} \) values that are sampled for use in computing scattering kinematics.

### 6.3 Implementation of On-the-Fly Broadening

Before presenting the procedure for stochastically sampling a temperature-dependent scattering kernel, it is illustrative to show how deterministic broadening can be performed and the results of that process. Starting from Equation (6.1), without loss of generality, the \( \mu_{\text{out}} \)-integrated cross section, \( \sigma_x(0, v_{\text{rel}}) \), can be expanded in \( \mu_{\text{out}} \) giving

\[
v_n \sigma_x(T, v_n) = \int_{\vec{v}_t} d\vec{v}_t \int_{-1}^1 d\mu_{\text{out}} V(T, \vec{v}_t) v_{\text{rel}} P(\mu_{\text{out}} | v_{\text{rel}}) \sigma_x(0, v_{\text{rel}}).
\]  

(6.3)

Dividing by \( v_n \sigma_x(T, v_n) \), which is constant with respect to the integration variables, leaves a definite integral over the distributions of all possible target velocities and scattering cosines that computes to unity. This means that the integrand and a normalization constant constitute, by definition, a probability density function for the consistent, Doppler broadened double-differential reaction kernel,

\[
P(\vec{v}_t, \mu_{\text{out}} | v_n) = \frac{1}{v_n \sigma_x(T, v_n)} V(T, \vec{v}_t) v_{\text{rel}} P(\mu_{\text{out}} | v_{\text{rel}}) \sigma_x(0, v_{\text{rel}}).
\]  

(6.4)

Now, for a given incident neutron energy and material temperature, integrating over \( \vec{v}_t \) gives the broadened scattering cosine distribution. In Figures 6.5 and 6.6 the broadened distributions at temperatures of \( 10^3 \) K and \( 10^8 \) K, respectively, are plotted along with the 0 K distribution for an incident energy of 0.7 MeV.\(^1\) It is clear that the \( 10^3 \) K kernel is distorted very little whereas the \( 10^8 \) K kernel exhibits significant Doppler effects.

\(^1\)This value is chosen for its proximity to many nuclides’ most probable fission neutron energy.
Figure 6.5: ENDF/B-VII.1 $^{56}$Fe elastic scattering cosine distributions at 0.7 MeV

Figure 6.6: ENDF/B-VII.1 $^{56}$Fe elastic scattering cosine distributions at 0.7 MeV
Kernels broadened with deterministic methods are only exact at the precise temperature to which they are broadened. This would lead to a dramatic increase in secondary distribution data memory requirements if multiple temperatures must be considered. However, Equation (6.4) can also be sampled using an entirely equivalent stochastic algorithm — one which preserves consistency between Doppler broadened cross sections, sampled target velocities, and sampled secondary distributions. Further, because only 0 K secondary distribution data is required, there is no computer memory penalty.

First, cross sections are Doppler broadened at all available energies. Broadening must be performed at all energies so that thermal target motion can be consistently accounted for when sampling secondary distributions which can become strongly anisotropic at energies above typical Doppler broadening cutoff energies.

Next, a target velocity is sampled in any elastic scattering event, at all energies with Doppler broadened cross section data. Proceeding with the constant 0 K elastic scattering cross section assumption and an ideal gas model for the distribution of target velocities, Equation (6.1) can be recast as a joint probability distribution for \( \mu_{\text{in}} \) and \( v_t \),

\[
P(v_t, \mu_{\text{in}} \mid v_n) \propto v_{\text{rel}} M(T, v_t).
\]

(6.5)

The sampling of Equation (6.5) can be simplified through the inclusion of canceling \( v_n + v_t \) terms which allows the distribution to be rewritten as

\[
P(v_t, \mu_{\text{in}} \mid v_n) = C \frac{v_{\text{rel}}}{v_n + v_t} \left[ v_n v_t^2 e^{-\beta^2 v_t^2} + v_t^3 e^{-\beta^2 v_t^2} \right];
\]

(6.6)

\[
C = \frac{2\beta^3}{v_n \sqrt{\pi}}
\]

where \( C \) is a normalization constant that is independent of the target velocity. Then,

\[\text{NJOY2012.50 is used to produce the Doppler broadened cross sections used in this work.}\]
\( \mu_{\text{in}} \) is sampled uniformly and \( v_t \) is obtained by sampling the distribution defined by the bracketed terms in Equation (6.6) [104]. The sample target velocity specified by \( \mu_{\text{in}} \) and \( v_t \) is accepted with a probability equal to the ratio

\[
R = \frac{v_{\text{rel}}}{v_n + v_t}, \tag{6.7}
\]

In order to account for the energy dependence of 0 K elastic scattering cross sections when sampling a target velocity, an additional criterion for rejecting the sample velocity — referred to as the Doppler broadening rejection correction (DBRC) — was proposed [108] and implemented [106].

Modifying Equation (6.6) by reintroducing the energy-dependent cross section term and adding canceling \( \sigma_{n}^{\text{MAX}}(T = 0) \) terms yields

\[
P(v_t, \mu_{\text{in}} \mid v_n) = C_{\text{DBRC}} \frac{\sigma_n(0, v_{\text{rel}})}{\sigma_{n}^{\text{MAX}}(T = 0)} \frac{v_{\text{rel}}}{v_n + v_t} \times (v_n v_t^2 e^{-\beta^2 v_t^2} + v_t^3 e^{-\beta^2 v_t^2});
\]

\[
C_{\text{DBRC}} = \frac{2 \beta^3 \sigma_{n}^{\text{MAX}}(T = 0)}{v_n \sqrt{\pi \sigma_n(T, v_n)}}, \tag{6.8}
\]

where \( \sigma_{n}^{\text{MAX}}(T = 0) \) is the maximum 0 K elastic scattering cross section on the interval of practically attainable \( v_{\text{rel}} \) values. Target velocity samples accepted after the Equation (6.7) rejection are subjected to the additional DBRC criterion and accepted with a probability of

\[
P_{\text{DBRC}} = \frac{\sigma_n(0, v_{\text{rel}})}{\sigma_{n}^{\text{MAX}}(T = 0)}. \tag{6.9}
\]

Once accepted, the target velocity is used to sample an outgoing scattering cosine.
from the energy-dependent secondary angular distribution at the relative neutron-nucleus energy. By increasing the energy at which this rejection is applied, secondary angular distributions which can vary significantly with energy are encountered. This phenomenon is not usually encountered in typical applications of the DBRC algorithm in the epithermal energy range which are primarily concerned with sampling a target velocity for the purpose of computing scattering kinematics. Scattering distributions are often quite isotropic at these energies.

6.3.1 Numerical Code Verification

Figure 6.7: Broadened ENDF/B-VII.1 $^{56}$Fe elastic scattering cosine distributions

In order to verify the implementation of the stochastic sampling procedure in OpenMC, the $^{56}$Fe elastic scattering cosine distribution is computed at an incident neutron energy of 0.7 MeV and a temperature of $10^7$ K using both deterministic integration and
the newly-implemented sampling scheme. Both distributions are plotted in Figure 6.7 which shows excellent agreement between the two.

6.4 Results and Analysis

Additional simulations are run in order to more fully quantify the effects of Doppler broadening on elastic scattering kernels. In each one, the results obtained with the exact, fully-consistent, broadened kernel are compared to those obtained with the methods and parameters that are typical of a state-of-the-art transport code. In the latter case, cross sections are broadened according to the default NJOY2012.50 behavior; constant cross section ideal gas scattering is modeled below $400k_B T$; and resonance elastic scattering is modeled below 1 keV and supercedes ideal gas scattering where the energy intervals overlap. As a consequence, secondary distribution Doppler broadening is also neglected above the greater value of $400k_B T$ and 1 keV.

First, elastic scattering kernels at 0.7 MeV are computed and plotted as a function of scattering cosine and relative neutron-nucleus energy. The reference and fully-broadened $10^7$ K distributions are found in Figures 6.8 and 6.9, respectively. The neglect of Doppler effects with respect to the secondary distribution in the reference case is indicated by the kernel’s existence at a single relative energy. With no target motion, all events occur at 0.7 MeV. This is manifestly different than the behavior displayed in the broadened case.

Up to this point, all results have been produced for a single incident neutron energy. To investigate the possibility that differences between the reference and broadened cases cancel out when a range of incident energies is considered, neutron slowing down spectra are calculated using a Watt fission spectrum source. Figures 6.10 and 6.11 show, respectively, the spectra computed in infinite media of $^{56}$Fe and $^{208}$Pb at $10^3$ K using the ECCO-2000 energy group structure. There appears to be little difference between the reference and exact cases.
Figure 6.8: ENDF/B-VII.1 $^{56}$Fe elastic scattering kernel, reference

Figure 6.9: ENDF/B-VII.1 $^{56}$Fe elastic scattering kernel, broadened
Figure 6.10: Infinite medium $^{56}$Fe slowing down flux spectra

Figure 6.11: Infinite medium $^{208}$Pb slowing down flux spectra
The flux spectra computed in the same systems, except at $10^8$ K, are shown in Figures 6.12 and 6.13, respectively. There are marked differences between the flux spectra, frequently $>10\%$ and approaching or exceeding $\sim 100\%$ in the vicinity of large scattering resonances where upscattering effects are significant. This is particularly evident near the 27.8 keV $^{56}\text{Fe}$ resonance where the flux spectra differ by nearly an order of magnitude over an interval of $\sim 10$ keV.

![Graph](image)

**Figure 6.12**: Infinite medium $^{56}\text{Fe}$ slowing down flux spectra

The significantly harder spectra of the broadened cases is an interesting consequence of resonance scattering leading to the occurrence of more interactions at relative neutron-nucleus energies near resonance energies where secondary distributions are more forward-peaked. Resonance scattering also results in increased scattering with target nuclei sampled from the higher energy tail of the Maxwell-Boltzmann distribution. On average, both of these phenomena lead to increased secondary neutron energies and harder spectra.
However, these hardened spectra are observed in the $10^8$ K cases and not at $10^3$ K. This behavior is expected if one considers the underlying cause of Doppler effects. The thermal motion of a nucleus creates a relative neutron-nucleus energy that results in the neutron experiencing a cross section and secondary distribution at an energy other than its laboratory energy. If this is to have an impact on calculated results, the cross section or secondary distribution must vary over the range of relative energies that are made possible due to target motion. This situation occurs when resonances are narrow or secondary distributions shift with respect to $16k_B T$, the maximum target energy. Clearly, this is more often the case at elevated temperatures.
6.5 Conclusions

A methodology for the consistent modeling of the effects of thermal target motion on effective cross sections, scattering kinematics, and secondary distributions in continuous-energy Monte Carlo transport simulations is presented. Only the 0 K secondary distribution data, which is also used in standard treatments, is required which means that there is no additional computer memory burden. Verification of the stochastic sampling process with a deterministic reference result is performed and shows excellent agreement between the two approaches. The methodology is also used to sample temperature-dependent elastic scattering kernels in neutron slowing down calculations. Differences between flux spectra computed with the consistent, Doppler broadened kernels and those computed using methods commonly employed in Monte Carlo codes can be significant at astrophysical temperatures but are negligible at power reactor operating temperatures. Future work should be directed at determining whether or not target motion effects are also negligible if secondary distributions are modeled as having detailed resonance structure rather than the smooth variation in energy that is typical of the current generation of nuclear data evaluations. With more rapid variations in energy, it is possible that secondary distribution effects will manifest themselves at lower temperatures. The methodology is also extensible to other reactions. This should be explored, particularly in the context of threshold reactions such as level inelastic scattering. Additionally, performance improvements can likely be had by switching from the DBRC algorithm to an accelerated rejection sampling technique [109].
Chapter 7

Summary and Conclusions

Computational methods for on-the-fly representation and processing of nuclear data within Monte Carlo neutron transport simulations of intermediate and fast spectrum systems are developed and implemented in a continuous-energy Monte Carlo code. A capability to compute temperature-dependent unresolved resonance region (URR) cross sections directly from zero-temperature average resonance parameters is presented as is an on-the-fly probability table interpolation scheme. Additional methods for calculating multi-level URR elastic scattering cross sections and generating resonance structure in competitive reaction cross sections are implemented. The main underlying assumption of the probability table method is also tested by comparing the results it yields with results that are averaged over many independent simulations, each using a single, independent realization of URR resonance parameters throughout. Finally, a procedure for consistent on-the-fly sampling of temperature-dependent neutron reaction kernels which requires no additional secondary distribution data is presented. The principal contributions deriving from the development of these methods and their subsequent use in analyses of intermediate and fast spectrum systems are

- a partial resolution of a longstanding discrepancy between experiment
and calculation results for a well-known fast critical assembly

- demonstration that coarse temperature mesh interpolation of probability table data is suitable for the simulation of systems having detailed temperature distributions

- quantitative validation that level-level interference effects in URR elastic scattering cross sections are negligible in many cases of interest

- evidence that neglecting cross section structure for reactions other than elastic scattering, capture, and fission can lead to non-negligible, unconservative biases in criticality safety calculations

- findings that unknown URR resonance structure significantly increases the uncertainty to which multiplication factor results can be stated

- exhibition of the strong impact that Doppler effects can have on secondary angular distributions in elastic scattering events at astrophysical temperatures

Sections 7.1 to 7.5 briefly describe each of the computational methods that are implemented along with key results obtained in analyses performed with each method. Implications of these results and paths for future research are also discussed.

### 7.1 Direct Cross Section Calculation

A process for computing temperature-dependent URR cross sections directly from the 0 K average resonance parameters provided in ENDF-6 nuclear data evaluations is developed. Because cross sections are computed continuously in the $E_n$, $T$, and $\sigma_t$ variables, simulations utilizing on-the-fly cross sections can be used in the benchmarking of the discrete, processed probability table data that is typically used to
model URR resonance structure in state-of-the-art transport codes. Also, because cross sections are computed directly from evaluated nuclear data within the transport simulation, there is no need for any pre-processing of URR resonance parameter data. This feature will allow evaluators to conveniently benchmark URR evaluations without the need for a nuclear data processing code. Applying the capability in this fashion yielded the results shown in Figure 7.1. It is clear that extending the upper bound of the $^{238}$U URR evaluation beyond the value used in all major evaluated nuclear data libraries leads to a noticeable positive reactivity effect in simulations of the Zero Energy Breeder Reactor Assembly (ZEBRA). This observation is significant because the positive reactivity helps to partially resolve the longstanding discrepancy between simulations and experiment for this system. The upward trend in $k_\infty$ also indicates that the extension of the URR evaluation to still higher energies may resolve the discrepancy further.

Figure 7.1: Variation of ZEBRA $k_\infty$ with $^{238}$U upper URR energy bound
The probability table method [64] has become the standard approach for modeling URR resonance structure in Monte Carlo simulations. However, typical treatments require the processing of evaluated nuclear data into discrete probability table data at each temperature that is present in a simulation, or statistical interpolation between data at discrete temperatures. If detailed spatial or temporal temperature variations must be simulated, generating data at discrete temperatures could lead to excessive memory requirements. However, at a single temperature, using probability table data can be much faster than the on-the-fly calculations in Chapter 2. The need for the fast calculation of temperature-dependent cross sections with manageable memory requirements leads to the probability table interpolation scheme presented in Chapter 3. It proceeds by generating cross section magnitude bands that are equiprobable.
across an $E_n$-$T$ mesh in a pre-processing step. Then, when a cross section value is needed in a simulation, a band is sampled and then interpolated in $E_n$ and $T$. With data generated at only 3 temperatures in the range from 293.6 K to 2500 K, interpolated probability table cross sections are shown to reproduce very well the reference $k_{\text{eff}}$ values for the Big Ten critical assembly that are computed with the continuous-temperature on-the-fly method. Figure 7.2 shows the RMS $\Delta k_{\text{eff}}$ values obtained using different temperature-cross section interpolation schemes in simulations of Big Ten at each of 21 temperatures spanning 350–2350 K at 100 K intervals. The relatively low RMS $\Delta k_{\text{eff}}$ values attained with very few temperature points and multiple interpolation schemes suggest that the interpolation of coarse-mesh probability table data in temperature may be suitable for simulations of intermediate and fast spectrum systems having detailed temperature variation in space and/or time.

7.3 Multi-Level and Competitive Reaction Resonance Effects

In computing probability tables, or otherwise generating cross sections in the URR, it is common practice to use the single-level Breit-Wigner (SLBW) resonance formalism. It is known that SLBW cross sections can differ significantly from cross sections computed with a multi-level formalism that accounts for level-level interference effects. A capability to compute temperature-dependent multi-level Breit-Wigner (MLBW) elastic scattering cross sections on-the-fly is implemented and used in a simulation of ZEBRA to generate the results in Table 7.1 which show a negligible departure from the SLBW $k_{\infty}$ value.

In examining Figure 7.3, it can be seen that the flux spectra computed with SLBW and MLBW cross sections are in very close agreement. This indicates that the use of the SLBW formalism for reconstructing URR resonance structure appears to be an
Table 7.1: ZEBRA $k_\infty$

<table>
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<th>URR Cross Sections</th>
<th>$k_{\text{eff}}$</th>
<th>$1\sigma$</th>
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<tr>
<td>Energy-averaged</td>
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<td>On-the-fly SLBW</td>
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<td>On-the-fly MLBW</td>
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</tbody>
</table>

acceptable approximation in simulations of systems with a fission spectrum source. For a shielding calculation with a monoenergetic source, this may very well not be the case as SLBW and MLBW cross sections could differ significantly at the specific incident source energy. Extension of the MLBW implementation beyond the ENDF-6 format version to account for level-level interference effects in the cross sections for reactions other than elastic scattering can be considered in future work.

Figure 7.3: ZEBRA flux spectra

Another approximation commonly-employed when modeling URR resonance struc-
Table 7.2: ZEBRA $k_\infty$

<table>
<thead>
<tr>
<th>URR Cross Sections</th>
<th>Competitive Cross Section</th>
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<th>1σ</th>
</tr>
</thead>
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<td>Energy-averaged</td>
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<td>0.00005</td>
</tr>
<tr>
<td>On-the-fly</td>
<td>Energy-averaged</td>
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<td>0.00006</td>
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<tr>
<td>On-the-fly</td>
<td>Resonance structure</td>
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<td>0.00005</td>
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</table>

ture is the use of energy-averaged cross section values for so-called competitive reactions (i.e., reactions other than elastic scattering, capture, and fission) despite the existence of resonance structure in these reactions’ cross sections. In order to determine the effects of this approximation, a capability to compute structured cross sections for one competitive reaction is implemented and used in simulations of ZEBRA. Comparing the $k_\infty$ values in Table 7.2, an unconservative, negative reactivity bias of $\sim 150$ pcm is observed when competitive resonance structure is neglected. The non-negligible effect of competitive resonance structure on flux spectra can be seen in Figure 7.4. These results illustrate the need for using competitive reaction partial widths to generate structured URR cross sections in criticality safety calculations. If future nuclear data evaluations provide average URR partial widths for multiple competitive reactions, the effects of modeling the resonance structure of each of those reactions should be investigated.

7.4 Independent Resonance Realizations by Simulation

Another principal assumption underlying both probability table and direct on-the-fly cross section calculations is that URR self-shielding effects can be adequately accounted for in Monte Carlo simulations by generating a new realization of URR resonance structure at each event. This is unphysical as there is a single, unchanging realization of resonance structure that exists in nature. In order to quantify the effects of this assumption on calculated results, a capability to generate a single re-
eralization of URR resonance structure and use that realization throughout an entire transport simulation is implemented. By running multiple independent simulations, each using a single, independent URR realization throughout, more rigorous expected value tallies can be computed by averaging over the independent results. Also, the spread of results that is attributable to unknown URR resonance structure can be determined by comparing the range of independent results with the range that is expected based on statistical uncertainty alone. Such information is not available when using probability table or on-the-fly calculations. Figure 7.5 illustrates a middle 95% $k_\infty$ range of nearly 400 pcm in 250 independent ZEBRA simulations. And because this uncertainty is induced by unknown resonance parameters, rather than statistics alone, it cannot be eliminated, or even reduced, by simulating more neutron histories. This URR uncertainty represents a new, significant increase of the lower bound on the uncertainty to which intermediate and fast spectrum critical assembly multiplica-
tion factors can be calculated. Additional work should be aimed at quantifying this uncertainty in simulations of more realistic fast reactor models. Along with this, the effect of URR uncertainties on other parameters of interest, such as Doppler reactivity coefficients, should be investigated.

### 7.5 Secondary Distribution Doppler Broadening

In modeling the angular distributions of secondary neutrons, Doppler broadening effects are rarely accounted for. When they are, it is at lower energies where the distributions do not exhibit much energy dependence. A procedure for consistently treating the effects of a non-zero target velocity on effective cross sections, scattering kinematics, and secondary angular distributions is developed and used to quantify...
the effects of neglecting the Doppler broadening of elastic scattering kernels at intermediate and fast neutron energies. $^{56}$Fe neutron slowing down spectra computed with both consistently Doppler broadened kernels and the methods and parameters which are representative of state-of-the-art Monte Carlo transport codes are plotted in Figure 7.6. A significant hardening of the spectrum is observed in the $10^8$ K Doppler broadened case due to some combination of preferential neutron scattering from energetic nuclei and an increased forward-peaked scattering rate. This reaction kernel broadening procedure is extensible to other reactions and may find applications in the modeling of threshold broadening which is currently neglected by state-of-the-art processing and transport codes. Additionally, future work should be directed at determining whether or not Doppler effects are also negligible if secondary angular distributions are modeled as having detailed resonance structure rather than the smooth variation in energy that is typical of the current generation of nuclear data evaluations. With more rapid variations in energy, it is possible that secondary distribution effects will manifest themselves at lower temperatures.
## Appendix A

### ENDF/B-VII.1 URR Nuclides

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<tr>
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<tr>
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<td>1.000000E+4</td>
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<tr>
<td>U-241</td>
<td>1.025000E+2</td>
<td>1.000000E+4</td>
</tr>
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<td>Upper energy bound [eV]</td>
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<tr>
<td>---------</td>
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<td>------------------------</td>
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<tr>
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<td>1.000000E+4</td>
</tr>
<tr>
<td>Np-237</td>
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<tr>
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<td>2.728320E+4</td>
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<td>Am-243</td>
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<td>4.237510E+4</td>
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<td>4.000000E+4</td>
</tr>
<tr>
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<td>1.000000E+5</td>
</tr>
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<td>4.000000E+4</td>
</tr>
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<td>Cm-246</td>
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<td>1.400000E+5</td>
</tr>
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<td>Cm-247</td>
<td>6.000000E+2</td>
<td>4.000000E+4</td>
</tr>
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<td>Cm-248</td>
<td>1.500000E+3</td>
<td>2.000000E+5</td>
</tr>
<tr>
<td>Cm-250</td>
<td>1.500000E+2</td>
<td>2.000000E+5</td>
</tr>
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<td>Bk-249</td>
<td>6.000000E+1</td>
<td>3.000000E+4</td>
</tr>
<tr>
<td>Cf-249</td>
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<tr>
<td>Cf-251</td>
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<tr>
<td>Cf-252</td>
<td>1.000000E+3</td>
<td>1.500000E+5</td>
</tr>
</tbody>
</table>
Appendix B

Model Descriptions

B.1 Big Ten

Big Ten is a large, cylindrical, split-table critical assembly designed to have a spectrum enabling experiments relevant to fast reactor physics. The assembly consists of a homogeneous 10% enriched uranium core surrounded by alternating plates of natural uranium and 93% enriched uranium to simulate more 10% enriched metal. These plates are then surrounded by a depleted uranium reflector [82]. The experimental setup is shown in Figure B.1.

All simulations of the Big Ten assembly for which results are reported in this thesis are performed using the IEU-MET-FAST-007, case 4 benchmark model from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [85]. The only isotopes present in this benchmark model of Big Ten are \(^{234}\text{U},^{235}\text{U},^{236}\text{U},\) and \(^{238}\text{U}\). The benchmark \(k_{\text{eff}}\) value is 1.00490 ± 0.00080.
Figure B.1: Big Ten critical experiment setup
B.1.1 OpenMC Input

B.1.1.1 Materials

```xml
<?xml version="1.0"?>
<materials>

<default_xs>80c</default_xs>

<!-- Homogenized HEU, Natural U, and Voids -->
<material id="1">
    <density units="sum" />
    <nuclide name="U-234" ao="5.4058e-05" />
    <nuclide name="U-235" ao="4.9831e-03" />
    <nuclide name="U-236" ao="1.3733e-05" />
    <nuclide name="U-238" ao="4.3108e-02" />
</material>

<!-- Intermediate Enriched Uranium (10 wt%) -->
<material id="2">
    <density units="sum" />
    <nuclide name="U-234" ao="2.4761e-05" />
    <nuclide name="U-235" ao="4.8461e-03" />
    <nuclide name="U-236" ao="1.3348e-05" />
    <nuclide name="U-238" ao="4.2695e-02" />
</material>

<!-- Natural Uranium -->
<material id="3">
    <density units="sum" />
    <nuclide name="U-234" ao="2.6518e-06" />
    <nuclide name="U-235" ao="3.4701e-04" />
    <nuclide name="U-238" ao="4.7846e-02" />
</material>
```

185
32 <!-- Depleted Uranium -->
33 <material id="4">
34   <density units="sum"/>
35   <nuclide name="U-234" ao="2.8672e-07"/>
36   <nuclide name="U-235" ao="1.0058e-04"/>
37   <nuclide name="U-236" ao="1.1468e-06"/>
38   <nuclide name="U-238" ao="4.7677e-02"/>
39 </material>
40
41 </materials>

B.1.1.2 Geometry

1 <!-- html -->
2 <xml version="1.0"?
3 <geometry>
4   <surface id="1" type="z-cylinder" coeffs="0. 0. 2.25014"/>
5   <surface id="2" type="z-cylinder" coeffs="0. 0. 3.10996"/>
6   <surface id="3" type="z-cylinder" coeffs="0. 0. 7.62000"/>
7   <surface id="4" type="z-cylinder" coeffs="0. 0. 12.54604"/>
8   <surface id="5" type="z-cylinder" coeffs="0. 0. 26.67000"/>
9   <surface id="6" type="z-cylinder" coeffs="0. 0. 41.91000" boundary="vacuum"/>
10  <surface id="7" type="z-plane" coeffs="-57.46750" boundary="vacuum"/>
11  <surface id="8" type="z-plane" coeffs="-41.73361"/>
12  <surface id="9" type="z-plane" coeffs="-38.24644"/>
13  <surface id="10" type="z-plane" coeffs="-22.39010"/>
14  <surface id="11" type="z-plane" coeffs="-4.35102"/>
15  <surface id="12" type="z-plane" coeffs="17.16665"/>
16  <surface id="13" type="z-plane" coeffs="23.81250"/>
17  <surface id="14" type="z-plane" coeffs="39.05250" boundary="vacuum"/>
18  <cell id="1" material="2" surfaces=" -3 8 -10"/>
19  <cell id="2" material="2" surfaces=" -4 10 -11"/>
20  <cell id="3" material="2" surfaces=" -2 11 -13"/>
21  <cell id="4" material="2" surfaces=" -1 13 -14"/>
B.2 ZEBRA

The Zero Energy Breeder Reactor Assembly (ZEBRA) is a facility for conducting critical experiments operated by the United Kingdom Atomic Energy Authority (UKAEA) from 1962 to 1982. A variety of experiments relevant to fast reactor physics were carried out at the facility, pictured in Figure B.2. One set of these experiments involved $k_\infty$ zone measurements consisting of a $\sim 0.3$ cm thick, $\sim 5$ cm$^2$ high-enriched uranium plate with $\sim 1$ cm of natural uranium plates above and below. The plates are stacked in a $\sim 0.2$ cm thick stainless steel sheath. The same plate stacking is repeated above and below the $k_\infty$ zone for the length of the $\sim 3$ m sheath and in adjacent sheaths. A region 11 sheaths in diameter is surrounded radially by a $^{235}$U driver region and reflected by natural uranium.

The model of this experiment used to generate the results reported in this thesis is the MIX-MET-FAST-008, core 8H benchmark model from ICSBEP. This is the same benchmark model as ZEBRA-FUND-RESR-001 from the International Reactor Physics Experiment Evaluation Project (IRPhEP) [110]. The benchmark $k_\infty$ value is $1.03000 \pm 0.00250$. 
B.2.1 OpenMC Input

B.2.1.1 Materials

```xml
<?xml version="1.0"?>
<materials>
  <default_xs>80c</default_xs>
  <!-- Enriched U metal (37.5 w/o) -->
  <material id="1">
    <density value="18.3890" units="g/cm3"/>
    <nuclide name="U-235" ao="1.7730e-02"/>
    <nuclide name="U-238" ao="2.8957e-02"/>
  </material>
</materials>
```
11  <nuclide name="C-Nat" ao="1.8452e-04" />
12  <nuclide name="O-16" ao="3.4618e-04" />
13  <nuclide name="O-17" ao="1.3160e-07" />
14  <nuclide name="Fe-54" ao="3.4794e-06" />
15  <nuclide name="Fe-56" ao="5.4618e-05" />
16  <nuclide name="Fe-57" ao="1.2614e-06" />
17  <nuclide name="Fe-58" ao="1.6787e-07" />
18  <nuclide name="Al-27" ao="4.1070e-05" />
19  <nuclide name="H-1" ao="4.3978e-05" />
20  <nuclide name="Si-28" ao="3.6390e-05" />
21  <nuclide name="Si-29" ao="1.8478e-06" />
22  <nuclide name="Si-30" ao="1.2181e-06" />
23  </material>
24
25  <!-- Natural U metal -->
26  <material id="2">
27    <density value="18.3227" units="g/cm3" />
28    <nuclide name="U-235" ao="3.3316e-04" />
29    <nuclide name="U-238" ao="4.5948e-02" />
30    <nuclide name="C-Nat" ao="4.9205e-04" />
31    <nuclide name="Fe-54" ao="6.1858e-06" />
32    <nuclide name="Fe-56" ao="9.7103e-05" />
33    <nuclide name="Fe-57" ao="2.2425e-06" />
34    <nuclide name="Fe-58" ao="2.9844e-07" />
35    <nuclide name="H-1" ao="4.3978e-05" />
36    <nuclide name="Si-28" ao="1.9408e-04" />
37    <nuclide name="Si-29" ao="9.8548e-06" />
38    <nuclide name="Si-30" ao="6.4963e-06" />
39  </material>
40
41  <!-- Sheath -->
42  <material id="3">
43    <density value="7.7681" units="g/cm3" />
44    <nuclide name="C-Nat" ao="7.7829e-04" />
45    <nuclide name="Fe-54" ao="3.3097e-03" />
46    <nuclide name="Fe-56" ao="5.1955e-02" />
<material>
  <nuclide name="Fe-57" ao="1.1999e-03" />
  <nuclide name="Fe-58" ao="1.5968e-04" />
  <nuclide name="Cr-50" ao="6.9985e-04" />
  <nuclide name="Cr-52" ao="1.3496e-02" />
  <nuclide name="Cr-53" ao="1.5303e-03" />
  <nuclide name="Cr-54" ao="3.8093e-04" />
  <nuclide name="Cu-63" ao="5.1084e-05" />
  <nuclide name="Cu-65" ao="2.2769e-05" />
  <nuclide name="Mo-92" ao="2.1718e-05" />
  <nuclide name="Mo-94" ao="1.3537e-05" />
  <nuclide name="Mo-95" ao="2.3299e-05" />
  <nuclide name="Mo-96" ao="2.4411e-05" />
  <nuclide name="Mo-97" ao="1.3976e-05" />
  <nuclide name="Mo-98" ao="2.3514e-05" />
  <nuclide name="Mo-100" ao="1.4094e-05" />
  <nuclide name="Mn-55" ao="1.1918e-03" />
  <nuclide name="Ni-58" ao="6.1297e-03" />
  <nuclide name="Ni-60" ao="2.3612e-03" />
  <nuclide name="Ni-61" ao="1.0264e-04" />
  <nuclide name="Ni-62" ao="3.2752e-04" />
  <nuclide name="Ni-64" ao="8.3342e-05" />
  <nuclide name="Al-27" ao="3.4646e-04" />
  <nuclide name="Ti-46" ao="2.4194e-05" />
  <nuclide name="Ti-47" ao="2.1819e-05" />
  <nuclide name="Ti-48" ao="2.1619e-04" />
  <nuclide name="Ti-49" ao="1.5865e-05" />
  <nuclide name="Ti-50" ao="1.5191e-05" />
  <nuclide name="H-1" ao="2.2714e-05" />
  <nuclide name="Si-28" ao="9.2219e-04" />
  <nuclide name="Si-29" ao="4.6826e-05" />
  <nuclide name="Si-30" ao="3.0868e-05" />
  <element name="V" ao="9.2127e-05" />
</material>
B.2.1.2 Geometry

1  <?xml version="1.0"?>
2  <geometry>
3  
4  <surface id="1" type="x-plane" coeffs="-2.62720" boundary="reflective" />
5  <surface id="2" type="x-plane" coeffs="-2.55100" />
6  <surface id="3" type="x-plane" coeffs="-2.53350" />
7  <surface id="4" type="x-plane" coeffs=" 2.53350" />
8  <surface id="5" type="x-plane" coeffs=" 2.55100" />
9  <surface id="6" type="x-plane" coeffs=" 2.62720" boundary="reflective" />
10 <surface id="7" type="y-plane" coeffs="-2.62720" boundary="reflective" />
11 <surface id="8" type="y-plane" coeffs="-2.55100" />
12 <surface id="9" type="y-plane" coeffs="-2.53350" />
13 <surface id="10" type="y-plane" coeffs=" 2.53350" />
14 <surface id="11" type="y-plane" coeffs=" 2.55100" />
15 <surface id="12" type="y-plane" coeffs=" 2.62720" boundary="reflective" />
16 <surface id="13" type="z-plane" coeffs="-1.11125" boundary="reflective" />
17 <surface id="14" type="z-plane" coeffs="-0.79375" />
18 <surface id="15" type="z-plane" coeffs="-0.47625" />
19 <surface id="16" type="z-plane" coeffs="-0.15875" />
20 <surface id="17" type="z-plane" coeffs=" 0.15875" />
21 <surface id="18" type="z-plane" coeffs=" 0.47625" />
22 <surface id="19" type="z-plane" coeffs=" 0.79375" />
23 <surface id="20" type="z-plane" coeffs=" 1.11125" boundary="reflective" />
24 
25  <cell id="1" material="2" surfaces="3 -4 9 -10 13 -14" />
26  <cell id="2" material="2" surfaces="3 -4 9 -10 14 -15" />
27  <cell id="3" material="2" surfaces="3 -4 9 -10 15 -16" />
28  <cell id="4" material="1" surfaces="3 -4 9 -10 16 -17" />
29  <cell id="5" material="2" surfaces="3 -4 9 -10 17 -18" />
30  <cell id="6" material="2" surfaces="3 -4 9 -10 18 -19" />
31  <cell id="7" material="2" surfaces="3 -4 9 -10 19 -20" />
32  <cell id="8" material="void" surfaces="2 -3 8 -11 13 -20" />
33  <cell id="9" material="void" surfaces="3 -4 8 -9 13 -20" />
34  <cell id="10" material="void" surfaces="4 -5 8 -11 13 -20" />

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B.3 LWR Pin Cell

The beginning of core (BOC), hot zero-power (HZP) pin cell results come from simulations of a pressurized-water reactor pin cell model taken from the Benchmark for Evaluation and Validation of Reactor Simulations (BEAVRS) [111]. It consists of fresh UO$_2$ fuel, a helium gap, Zircaloy-4 clad, and light-water moderator all at 600 K.

B.3.1 OpenMC Input

B.3.1.1 Materials

```xml
<materials>
    <default_xs>81c</default_xs>
    <material id="1">
        <density value="10.30187" units="g/cc" />
        <nuclide name="U-234" xs="81c" ao="5.7988e-06" />
        <nuclide name="U-235" xs="81c" ao="7.2176e-04" />
        <nuclide name="U-238" xs="81c" ao="2.2254e-02" />
    </material>
</materials>
```
<nuclide name="O-16" xs="81c" ao="4.5851e-02" />
<nuclide name="O-17" xs="81c" ao="1.1169e-04" />
</material>

<!-- Helium Gap at 600 K -->
<material id=" 2">
<density value="0.001598" units="g/cc" />
<nuclide name="He-4" xs="81c" ao="2.4044e-04" />
</material>

<!-- Zircaloy-4 at 600 K -->
<material id=" 3">
<density value="6.55" units="g/cc" />
<nuclide name="O-16" xs="81c" ao="3.0743e-04" />
<nuclide name="O-17" xs="81c" ao="7.4887e-07" />
<nuclide name="Cr-50" xs="81c" ao="3.2962e-06" />
<nuclide name="Cr-52" xs="81c" ao="6.3564e-05" />
<nuclide name="Cr-53" xs="81c" ao="7.2076e-06" />
<nuclide name="Cr-54" xs="81c" ao="1.7941e-06" />
<nuclide name="Fe-54" xs="81c" ao="8.6699e-06" />
<nuclide name="Fe-56" xs="81c" ao="1.3610e-04" />
<nuclide name="Fe-57" xs="81c" ao="3.1431e-06" />
<nuclide name="Fe-58" xs="81c" ao="4.1829e-07" />
<nuclide name="Zr-90" xs="81c" ao="2.1827e-02" />
<nuclide name="Zr-91" xs="81c" ao="4.7600e-03" />
<nuclide name="Zr-92" xs="81c" ao="7.2758e-03" />
<nuclide name="Zr-94" xs="81c" ao="7.3734e-03" />
<nuclide name="Zr-96" xs="81c" ao="1.1879e-03" />
<nuclide name="Sn-112" xs="81c" ao="4.6735e-06" />
<nuclide name="Sn-114" xs="81c" ao="3.1799e-06" />
<nuclide name="Sn-115" xs="81c" ao="1.6381e-06" />
<nuclide name="Sn-116" xs="81c" ao="7.0055e-05" />
<nuclide name="Sn-117" xs="81c" ao="3.7003e-05" />
<nuclide name="Sn-118" xs="81c" ao="1.1669e-04" />
<nuclide name="Sn-119" xs="81c" ao="4.1387e-05" />
<nuclide name="Sn-120" xs="81c" ao="1.5697e-04" />
B.3.1.2 Geometry

<xml version="1.0" encoding="UTF-8"?>
<geometry>
  <surface id="1" type="z-cylinder" coeffs="0.0 0.0 0.392180"/>
  <surface id="2" type="z-cylinder" coeffs="0.0 0.0 0.400050"/>
  <surface id="3" type="z-cylinder" coeffs="0.0 0.0 0.457200"/>
  <surface id="4" type="x-plane" coeffs="-0.62992" boundary="reflective"/>
  <surface id="5" type="x-plane" coeffs="0.62992" boundary="reflective"/>
  <surface id="6" type="y-plane" coeffs="-0.62992" boundary="reflective"/>
  <surface id="7" type="y-plane" coeffs="0.62992" boundary="reflective"/>
  <surface id="8" type="z-plane" coeffs="-183.0" boundary="reflective"/>
  <surface id="9" type="z-plane" coeffs="183.0" boundary="reflective"/>
  <cell id="1" universe="0" material="1" surfaces="-1 8 -9"/>
  <cell id="2" universe="0" material="2" surfaces="1 -2 8 -9"/>
  <cell id="3" universe="0" material="3" surfaces="2 -3 8 -9"/>
</geometry>
B.4 TWR Unit Cell

The traveling wave reactor (TWR) unit cell model that is simulated consists of a homogeneous, infinite medium with an isotopic composition that is representative of a generic TWR [112]. There are no fission products and significant quantities of $^{238}$U. The complete isotopic composition is given in Table B.1.

Table B.1: TWR unit cell isotopic composition

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>Density [atoms/b-cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Am-241</td>
<td>2.59872E-06</td>
</tr>
<tr>
<td>Am-242</td>
<td>1.24375E-07</td>
</tr>
<tr>
<td>Am-243</td>
<td>1.19103E-07</td>
</tr>
<tr>
<td>B-10</td>
<td>1.00000E-15</td>
</tr>
<tr>
<td>B-11</td>
<td>1.00000E-15</td>
</tr>
<tr>
<td>C</td>
<td>1.27502E-04</td>
</tr>
<tr>
<td>Cm-242</td>
<td>1.07955E-07</td>
</tr>
<tr>
<td>Cm-243</td>
<td>3.25679E-09</td>
</tr>
<tr>
<td>Cm-244</td>
<td>1.92010E-08</td>
</tr>
<tr>
<td>Cm-245</td>
<td>1.59285E-09</td>
</tr>
<tr>
<td>Cm-246</td>
<td>6.02952E-11</td>
</tr>
<tr>
<td>Cm-247</td>
<td>1.02307E-12</td>
</tr>
<tr>
<td>Cr</td>
<td>1.76712E-03</td>
</tr>
<tr>
<td>Fe</td>
<td>1.15927E-02</td>
</tr>
<tr>
<td>Hf-174</td>
<td>1.00000E-15</td>
</tr>
<tr>
<td>Hf-176</td>
<td>1.00000E-15</td>
</tr>
<tr>
<td>Hf-177</td>
<td>1.00000E-15</td>
</tr>
</tbody>
</table>
Table B.1: TWR unit cell isotopic composition

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>Density [atoms/b-cm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hf-178</td>
<td>1.00000E-15</td>
</tr>
<tr>
<td>Hf-179</td>
<td>1.00000E-15</td>
</tr>
<tr>
<td>Hf-180</td>
<td>1.00000E-15</td>
</tr>
<tr>
<td>Mn-55</td>
<td>8.36244E-05</td>
</tr>
<tr>
<td>Mo</td>
<td>7.98116E-05</td>
</tr>
<tr>
<td>Na-23</td>
<td>6.03302E-03</td>
</tr>
<tr>
<td>Ni</td>
<td>6.52283E-05</td>
</tr>
<tr>
<td>Np-237</td>
<td>9.18861E-06</td>
</tr>
<tr>
<td>Np-238</td>
<td>7.20904E-09</td>
</tr>
<tr>
<td>Pu-236</td>
<td>8.76545E-11</td>
</tr>
<tr>
<td>Pu-238</td>
<td>3.98326E-06</td>
</tr>
<tr>
<td>Pu-239</td>
<td>1.02848E-03</td>
</tr>
<tr>
<td>Pu-240</td>
<td>1.80400E-04</td>
</tr>
<tr>
<td>Pu-241</td>
<td>1.45972E-05</td>
</tr>
<tr>
<td>Pu-242</td>
<td>1.70767E-06</td>
</tr>
<tr>
<td>Si</td>
<td>1.09052E-04</td>
</tr>
<tr>
<td>U-234</td>
<td>1.68738E-07</td>
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<tr>
<td>U-235</td>
<td>4.72861E-06</td>
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<tr>
<td>U-236</td>
<td>5.34379E-06</td>
</tr>
<tr>
<td>U-238</td>
<td>9.78903E-03</td>
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<tr>
<td>V</td>
<td>3.86925E-04</td>
</tr>
<tr>
<td>W-182</td>
<td>5.52516E-06</td>
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<tr>
<td>W-183</td>
<td>2.98355E-06</td>
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<tr>
<td>W-184</td>
<td>6.38823E-06</td>
</tr>
<tr>
<td>W-186</td>
<td>5.92733E-06</td>
</tr>
<tr>
<td>Zr</td>
<td>1.06093E-04</td>
</tr>
</tbody>
</table>
B.4.1 OpenMC Input

B.4.1.1 Materials

```xml
<?xml version="1.0"?>
<materials>
  <default_xs>82c</default_xs>
  <material id="1">
    <density units="sum" />
    <nuclide name="AM-241" ao="2.59872E-06"/>
    <nuclide name="AM-242" ao="1.24375E-07"/>
    <nuclide name="AM-243" ao="1.19103E-07"/>
    <nuclide name="AM-244" ao="1.19103E-07"/>
    <nuclide name="AM-245" ao="1.19103E-07"/>
    <nuclide name="AM-246" ao="1.19103E-07"/>
    <nuclide name="AM-247" ao="1.19103E-07"/>
    <nuclide name="B-10" ao="1.00000E-15"/>
    <nuclide name="B-11" ao="1.00000E-15"/>
    <element name="C" ao="1.27502E-04"/>
    <nuclide name="CM-242" ao="1.07955E-07"/>
    <nuclide name="CM-243" ao="3.25679E-09"/>
    <nuclide name="CM-244" ao="1.92010E-08"/>
    <nuclide name="CM-245" ao="1.59285E-09"/>
    <nuclide name="CM-246" ao="6.02952E-11"/>
    <nuclide name="CM-247" ao="1.02807E-12"/>
    <element name="CR" ao="1.76712E-03"/>
    <element name="FE" ao="1.15927E-02"/>
    <nuclide name="HF-174" ao="1.00000E-15"/>
    <nuclide name="HF-175" ao="1.00000E-15"/>
    <nuclide name="HF-177" ao="1.00000E-15"/>
    <nuclide name="HF-178" ao="1.00000E-15"/>
    <nuclide name="HF-179" ao="1.00000E-15"/>
    <nuclide name="HF-180" ao="1.00000E-15"/>
    <nuclide name="MN-55" ao="8.36244E-05"/>
    <element name="MO" ao="7.98116E-05"/>
    <nuclide name="NA-23" ao="6.03302E-03"/>
    <element name="NI" ao="6.52283E-05"/>
```
B.4.1.2 Geometry

<?xml version="1.0"?>
<geometry>
  <cell id="1">
    <material>1</material>
    <surfaces>-1 2 -3 4 -5 6</surfaces>
  </cell>
  <surface id="1" type="x-plane" coeffs="100.5" boundary='reflective'/>
  <surface id="2" type="x-plane" coeffs="-100.5" boundary='reflective'/>
</geometry>
B.5 Godiva

Godiva is a spherical, high-enriched uranium metal critical assembly formerly operated at Los Alamos National Laboratory [113]. With fission neutrons experiencing
little moderation from the heavy metal, the flux spectrum is extremely hard — more so than Big Ten or ZEBRA. The experimental setup is shown in Figure B.3.

All simulations of the Godiva assembly for which results are reported in this thesis are performed using the HEU-MET-FAST-001 solid metal benchmark model from ICSBEP. The only nuclides present in the model are $^{234}$U, $^{235}$U, and $^{238}$U. The benchmark $k_{\text{eff}}$ value is 1.00000 ± 0.00100.

### B.5.1 OpenMC Input

#### B.5.1.1 Materials

```xml
<materials>
  <default_xs>80c</default_xs>
  <!-- Godiva sphere at 18.74 g/cm3 -->
  <material id="1">
    <density units="sum" />
    <nuclide name="U-234" ao="4.9184e-04" />
    <nuclide name="U-235" ao="4.4994e-02" />
    <nuclide name="U-238" ao="2.4984e-03" />
  </material>
</materials>
```

#### B.5.1.2 Geometry

```xml
<geometry>
  <!-- Geometry details -->
</geometry>
```
<surface id="1" type="sphere" coeffs="0. 0. 0. 8.7407" boundary="vacuum" />
<cell id="1" material="1" surfaces="-1" />
</geometry>
Bibliography


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[96] A. V. Dralle, N. R. Candelore, and R. C. Gast. RCPL1- a program to prepare neutron and photon cross-section libraries for RCP01. Technical Report WAPD-


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