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On-the-fly Doppler broadening of unresolved resonance region cross sections

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ABSTRACT

Two methods for computing temperature-dependent unresolved resonance region cross sections on-the-fly within continuous-energy Monte Carlo neutron transport simulations are presented. The first method calculates Doppler broadened cross sections directly from zero-temperature average resonance parameters. In a simulation, at each event that requires cross section values, a realization of unresolved resonance parameters is generated about the desired energy and temperature-dependent single-level Breit-Wigner resonance cross sections are computed directly via the analytical $\psi - \chi$ Doppler integrals. The second method relies on the generation of equiprobable cross section magnitude bands on an energy-temperature mesh. Within a simulation, the bands are sampled and interpolated in energy and temperature to obtain cross section values on-the-fly. Both of the methods, as well as their underlying calculation procedures, are verified numerically in extensive code-to-code comparisons. Energy-dependent pointwise cross sections calculated with the newly-implemented procedures are shown to be in excellent agreement with those calculated by a widely-used nuclear data processing code. Relative differences at or below 0.1% are observed. Integral criticality benchmark results computed with the proposed methods are shown to reproduce those computed with a state-of-the-art processed nuclear data library very well. In simulations of fast spectrum systems which are highly-sensitive to the representation of cross section data in the unresolved region, *k*-eigenvalue and neutron flux spectra differences of <10 pcm and <1.0% are observed, respectively. The direct method is demonstrated to be well-suited to the calculation of reference solutions — against which results obtained with a discretized representation may be assessed — as a result of its treatment of the energy, temperature, and cross section magnitude variables as continuous. Also, because there is no pre-processed data to store (only temperature-independent average resonance parameters) the direct method is very memory-efficient. Typically, only a few kB of memory are needed to store all required unresolved region data for a single nuclide. However, depending on the details of a particular simulation, performing URR cross section calculations on-the-fly can significantly increase simulation times. Alternatively, the method of interpolating equiprobable probability bands is demonstrated to produce results that are as accurate as the direct reference solutions, to within arbitrary precision, with high computational efficiency in terms of memory requirements and simulation time. Analyses of a fast spectrum system show that interpolation on a coarse energy-temperature mesh can be used to reproduce reference *k*-eigenvalue results obtained with cross sections calculated continuously in energy and directly at an exact temperature to within <10 pcm. Probability band data on a mesh encompassing the range of temperatures relevant to reactor analysis usually require around 100 kB of memory per nuclide. Relative to the case in which probability table data generated at a single, desired temperature are used, minor increases in simulation times are observed when probability band interpolation is employed.

1. Introduction

The use of Monte Carlo particle transport codes, which, in

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principle, allow for physical and geometrical models of arbitrary fidelity, has historically been limited by the availability of computational resources. However, with the increased processing power of modern high-performance computing platforms, Monte Carlo methods are increasingly being considered for practical reactor analysis, rather than simply benchmarking purposes. Future research and development efforts will benefit from improved computational methods for the representation of nuclear data in Monte Carlo simulations of advanced reactor systems, many of which rely on intermediate or fast neutron spectra. For the simulation and analysis of fast reactors and critical assemblies, methods for the efficient, accurate calculation of Doppler broadened cross sections (i.e., effective, reaction rate-preserving cross sections which account for the energy-averaging effects of the thermal motion of target nuclei in a material at non-zero temperature) are of particular importance. And, while 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 Doppler broadening of thermal scattering data (Pavlou and Ji, 2014) and resolved resonance region (RRR) cross sections (Yesilyurt et al., 2012; Viitanen and Leppänen, 2012; Forget et al., 2014), the treatment of unresolved resonance region (URR) data has received less attention. The development of high-fidelity, computationally efficient methods for on-the-fly generation of temperature-dependent URR cross sections in Monte Carlo transport simulations is the focus of this work.

The remainder of this section gives brief introductions to important physical phenomena that characterize the unresolved resonance energy region and the computational methods that have previously been used to capture the effects of those phenomena in Monte Carlo simulations. Section 1.1 highlights defining characteristics of the URR as applicable to neutron transport simulations. In Section 1.2 the use of energy-averaged cross sections in the URR, and the pitfalls of this approach, are described. The probability table method for treating resonance cross section structure in the unresolved region is briefly outlined in Section 1.3. The direct calculation and probability band interpolation methods are detailed in Sections 2 and 3, respectively. Section 4 presents verification of the methods and the calculation procedures on which they are based with both differential cross section calculations and integral benchmark simulations. Results demonstrating the use of the direct method as a tool for validating probability band data are given in Section 5 as are analyses which show that probability band interpolation on a relatively coarse energy-temperature mesh is sufficient to reproduce reference results. Conclusions are stated in Section 6.

1.1. Unresolved resonance region

The URR spans the intermediate incident neutron energies between the highly-structured cross sections of the RRR and the broadly-fluctuating cross sections of the fast energy region. At these energies,[1] due to decreasing energy resolution with increasing incident energy in neutron cross section measurement experiments, individual resonances for a given nuclide cannot all be resolved 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 (i.e., nuclear level spacings and partial resonance reaction widths) and theoretical statistical distributions of those parameters (Foderaro, 1971).

1.2. Energy-averaged cross sections

Because the precise resonance structure of cross sections in the URR is unknown, cross section values at any specific energy are frequently unknown by orders of magnitude. While energy-averaged, expected value cross sections can be calculated from mean unresolved resonance parameter values and the statistical distributions of those values, it is generally not advisable to use these unshielded, infinite-dilute values in transport simulations. This is especially true for systems with an appreciable flux at URR energies.

In obtaining expected value cross sections, the resonance structure of the URR is smoothed. 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 under finite-dilution conditions. Thus, the impact of energy self-shielding is effectively neglected and reaction rates are over-predicted. The result is usually an under-prediction of k_{eff} (Mosteller and Little, 1999) due to increased URR absorption and increased downscattering to energies below the URR where the capture-to-fission ratio, α, is often higher. Further, the use of infinite-dilute cross sections requires the neglect of Doppler broadening effects which arise due to the resonance structure that is actually present in the URR. Therefore, high-fidelity simulations of fast reactor systems demand methods for modeling temperature-dependent URR resonance cross sections.

1.3. Probability tables

In order to more faithfully account for resonance structure and the resulting energy self-shielding effects in the URR — a phenomenon that can account for hundreds of pcm in reactivity in intermediate and fast spectrum systems — the probability table method was proposed (Levitt, 1972). It is now the most common procedure among production-level Monte Carlo transport codes for modeling URR cross section resonance structure. The method relies on the random sampling of tables of cross section bands that are pre-generated at discrete energies and temperatures on a nuclide-by-nuclide basis. At a given energy and temperature, each band is characterized by its probability of being sampled, a total cross section magnitude, and partial reaction cross section magnitudes that are conditional on the total cross section magnitude. Although the expected value cross sections at a given incident neutron energy are preserved in the limit of many samples, there is a distribution of discrete cross section magnitudes. It is this distribution that provides a more realistic model for URR energy self-shielding. The capability to generate probability tables is implemented in many established nuclear data processing codes such as NJOY (Macfarlane and Muir, 1994), PREPRO (Cullen, 2004), AMPX (Dunn and Greene, 2002), and CALENDF (Sublet et al., 2011). Certain practical considerations in implementing the probability table method are well-documented (Leal et al., 1989; Sutton and Brown, 1998; Dunn and Leal, 2004; MacFarlane and Kahler, 2010).

2. Direct calculation of cross sections

In this section an on-the-fly method for the direct calculation of URR cross sections is developed further from its preliminary

[1] The energy bounds of the URR depend on the nuclide with the onset coming at lower energies for nuclides having a higher density of nuclear levels (i.e., resonances).

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