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Creation of problem-dependent Doppler-broadened cross sections in the KENO Monte Carlo code ☆

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ABSTRACT

This paper introduces a quick method for improving the accuracy of Monte Carlo simulations by generating one- and two-dimensional cross sections at a user-defined temperature before performing transport calculations. A finite difference method is used to Doppler-broaden cross sections to the desired temperature, and unit-base interpolation is done to generate the probability distributions for double differential two-dimensional thermal moderator cross sections at any arbitrarily user-defined temperature. The accuracy of these methods is tested using a variety of contrived problems. In addition, various benchmarks at elevated temperatures are modeled, and results are compared with benchmark results. The problem-dependent cross sections are observed to produce eigenvalue estimates that are closer to the benchmark results than those without the problem-dependent cross sections.

1. Introduction

Cross-section files are generally provided in Evaluated Nuclear Data Format (ENDF) formatted data files (Trkov et al., 2011) that contain all of the necessary data to create continuous energy (CE) data libraries for use in a Monte Carlo calculation. To be useful, these ENDF data files are generally processed by a cross-section processing code such as AMPX (Dunn and Greene, 2002) or NJOY (MacFarlane and Muir, 2000) for use in a radiation transport code such as CE-KENO (Hollenbach et al., 2011). For one-dimensional cross sections, the data are usually provided at one temperature (designated as 0 K), and need to be Doppler-broadened to various temperatures before they can be used at reactor-level temperatures.

Exact Doppler-broadened cross sections can be done by the nuclear data-processing codes using Doppler broadening equations (Cullen et al., 1973); however, producing exact cross sections at a large number of temperatures would consume a significant amount of time and space, both in memory and on a hard disk. Therefore, cross-section libraries are generally only created at several different temperatures; for KENO, part of the SCALE code suite (ORNL, 2011), there are generally six temperatures created. For KENO in CE mode, if the temperature desired is not one of the pre-generated temperatures, then the closest temperature is used. A case containing materials that are 50 K away from a library temperature can produce significantly different results when compared with a case that is using the temperature-corrected cross sections.

Two-dimensional cross sections are generally provided for thermal moderators in order to account for crystalline effects encounted when neutrons are traveling at thermal speeds. Unlike the one-dimensional cross sections, the ENDF files are usually provided at a variety of temperatures. However, no Doppler broadening is done on these temperatures, so the end result is the same: If a temperature desired by the user is sufficiently far from the library temperatures, errors in the eigenvalue estimates can occur. Some previous work has been done to provide for on-the-fly (OTF) Doppler broadening of one-dimensional neutron cross sections (Yesilyurt et al., 2009; Yesilyurt et al., 2012; Brown et al., 2012; Martin et al., 2013; Trumbull, 2006) in other Monte Carlo codes. For example, MCNP6 (X-5 Monte Carlo Team, 2003) ships with a utility to generate fits to cross-section data so that cross sections can be calculated on-the-fly for any temperature as desired. KENO

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previously had no such capability to Doppler broaden cross sections.

In this paper two methods are discussed to temperature-correct the provided cross sections. A finite difference method is employed for the one-dimensional cross sections. This method is much faster than the exact Doppler-broadening method developed by Cullen and can use the data libraries that have already been created. For two-dimensional thermal moderator data, a simple unit-base interpolation scheme is used on the probability distributions of the double differential cross sections. By combining the aforementioned methods with temperature interpolation on the probability tables covering the unresolved resonance range (such as in Walsh et al. (2015)), KENO will have temperature-corrected neutron cross sections for all energy regions of interest (Hart et al., 2014).

2. One-dimensional method

For one-dimensional cross sections the approach to be implemented into KENO utilizes a finite-difference method similar to that used by SAMMY (Larson, 2008), which is well suited for resonance analysis and light water reactor (LWR) applications. This approach is based on the Leal-Hwang scattering method (Leal and Hwang, 1987), in which the Doppler broadened cross sections satisfy a heat equation of the form

$$\frac{\partial^2 F}{\partial u^2} = \frac{\partial F}{\partial \zeta}, \tag{1}$$

where F is the function of interest (in this case the cross section), u is the energy range, and ζ is the temperature. Then, because of the initial condition $F(u,0)$ for $-\infty < u < \infty$ and the boundary conditions $F(\infty,\zeta) = F(\infty,0)$ and $F(-\infty,\zeta) = F(-\infty,0)$, the function F can be calculated using the finite-difference method.

The application of the finite-difference method solves Eq. (1) by applying an explicit finite-difference formalism assuming constant meshes with $\delta u \equiv h$ and $\delta\zeta \equiv \gamma$. The first and second derivatives can then be expanded in a Taylor's series. Thus the explicit finite-difference equation for the function F at any u_i and ζ_{j+1} is

$$F_i^{j+1} = s\left(F_{i+1}^j + aF_i^j + F_{i-1}^j\right), \tag{2}$$

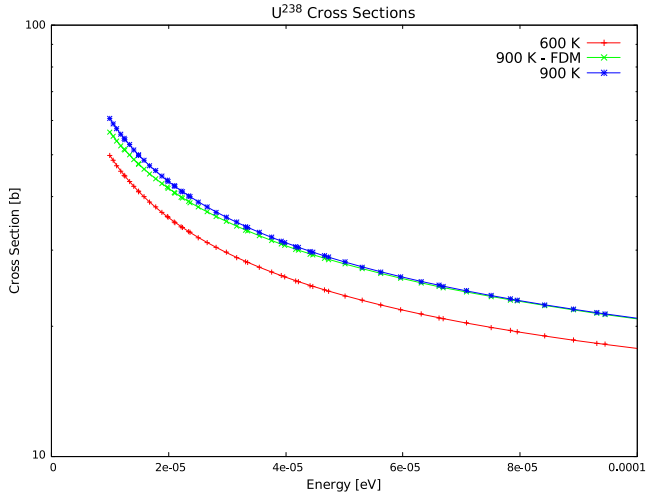
where $s \equiv \frac{\gamma}{h^2}$ and $a \equiv \frac{1-2s}{s}$. The finite-difference equation in Eq. (2) can be modified for nonuniform meshes as

$$F_i^{j+1} = s\left(aF_i^j + \frac{2(F_{i-1}^j \delta v_r + F_{i+1}^j \delta v_l)}{\delta v_r + \delta v_l}\right), \tag{3}$$

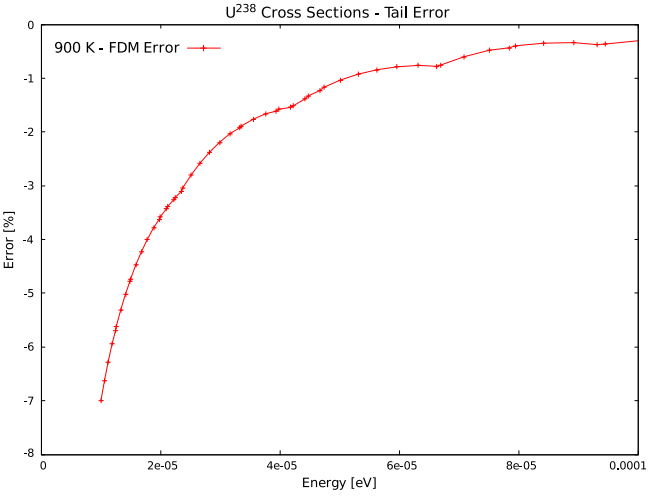
where $s \equiv \frac{\gamma}{\delta v_l \delta v_r}$, $a \equiv \frac{1-2s}{s}$, $\delta v_l = v_i - v_{i-1}$, $\delta v_r = v_{i+1} - v_i$, and v_i is the momentum at the ith grid point.

Selecting a ΔT that is small (such as 1 K) allows for agreement within 0.1% to reference cross sections across all energies except for very low and very high energies. The increase in error at the edges of the energy range is due to limitations in the finite-difference method. Because each element in the energy grid uses the surrounding elements to calculate the new value, the finite-difference method produces poor cross-section estimates when surrounding elements are inaccurate or do not exist. In an attempt to alleviate these errors, extra points can be added past the known energy range. This reduces the error for cross sections at very high and very low energies by extrapolating the known cross-section data but does not eliminate it completely.

Doppler broadening is controlled by the dbx parameter in KENO. By setting dbx to 1, the finite difference approach is enabled. Fig. 1 show the results of using the finite-difference method to obtain cross sections for the ^{238}U scattering reaction at 900 K near the low-energy tail. As previously discussed, the error in the tail region quickly disappears as one moves away from the energy boundary.



(a) Cross Sections



(b) Error

Fig. 1. ^{238}U scattering cross sections showing a tail.

As seen in Fig. 1, the error at the low-energy tail can approach 10%. Although the error probably has little effect on the results, it would be beneficial to try and minimize it. One solution is to use linear interpolation for the first five momentum points on the energy grid. Since there are no resonances in this extremely small energy range, doing so would not introduce any errors into the broadened cross sections. By using interpolation for the first ten points, the results from Fig. 1 using the FDM converge onto 900 K reference results.

An example of this approach is shown in Fig. 2 for ^{16}O. In Fig. 2 (a) there is a large error (approaching 10%) in the lower tail region. This contrasts sharply with the lack of error in the rest of the energy space, although there is a small error when the finite difference method is used in the resonances. In Fig. 2(b) the error has mostly disappeared and is less than 0.2% in the tail region. The rest of the energy range is mostly unaffected by the change.

Another problem may arise when dealing with isotopes that do not have a large resonance structure, are light, or have some other small irregularites. One example is ^{1}H in water, which contains no resonances and also isn't smoothly decreasing around 0.01 eV. This slight bump causes an instability in the finite difference method as