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Accelerated sampling of the free gas resonance elastic scattering kernel

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ABSTRACT

In this work, we present the derivation and investigation of a new Doppler broadening rejection sampling approach for the exact treatment of resonance elastic scattering in Monte Carlo neutron transport codes. Implemented in OpenMC, this method correctly accounts for the energy dependence of cross sections when treating the thermal motion of target nuclei in elastic scattering events. The method is verified against both stochastic and deterministic reference results in the literature for ^{238}U resonance scattering. Upscatter percentages and mean scattered energies calculated with the method are shown to agree well with the reference scattering kernel results. Additionally, pin cell and full core k_{eff} results calculated with this implementation of the exact resonance scattering kernel are shown to be in close agreement with those in the literature. The attractiveness of the method stems from its improvement upon a computationally expensive rejection sampling procedure employed by an earlier stochastic resonance scattering treatment. With no loss in accuracy, the accelerated sampling algorithm is shown to reduce overall runtime by 3–5% relative to the Doppler broadening rejection correction method for both pin cell and full core benchmark problems. This translates to a 30–40% reduction in runtime overhead.

1. Introduction

At sufficiently high incident neutron energies, elastic scattering can be accurately modeled with zero-velocity target nuclei. In the epithermal energy range, however, the thermal motion of target nuclei can have a significant effect on differential scattering kernels. These differences can, in turn, significantly effect macroscopic values such as the effective multiplication factor of a system. Therefore, it is important to have an accurate model for the kinematics of epithermal elastic scattering. Such a model requires that target velocities be drawn from the exact bivariate distribution in both speed and direction of flight (Ouisloumen and Sanchez, 1991).

Typically, stochastic treatments of epithermal elastic scattering make the assumption that the distribution of target speeds takes on that of an isotropic Maxwell–Boltzmann ideal gas. Historically, the procedure for sampling the target velocity distribution has also relied on the simplifying assumption that, in any given elastic scattering event, the cross section of the target nuclide is effectively constant over the narrow range of probable relative neutron speeds (Carter and Cashwell, 1975). This assumption leads to inadequate results for elastic scattering from heavy resonant nuclides which can exhibit rapid cross section variation over small energy intervals. Alternate stochastic treatments of resonance elastic scattering have been shown to correctly reproduce the exact scattering kernels. However, these methods give rise to appreciable decreases in computational efficiency.

It is the aim of this work to develop a resonance elastic scattering treatment that correctly reproduces exact scattering kernels and that also reduces the undesirable inefficiencies of previously proposed methods. The accelerated sampling method derived here is implemented in the OpenMC particle transport code (Romano and Forget, 2013). The method is verified through a comparison of computed scattering kernels with stochastic and deterministic reference literature results (Sunny et al., 2012; Trumbull and Fieno, 2013; Zoia et al., 2013; Ghrayeb et al., 2011). Comparisons of upscatter percentages and mean scattered energies for neutrons with incident energies near ^{238}U resonance energies – where resonance scattering effects are most pronounced – are presented. The results of pin cell and full core eigenvalue calculations are also analyzed. Sample target velocity rejection rates and runtimes are examined in order to assess the relative computational efficiency of the accelerated resonant target velocity sampling method proposed in this work.

2. Elastic scattering models

Correct treatment of the elastic scattering process is vital to the accuracy of reactor physics simulations. Multiple procedures, with varying degrees of physical fidelity, have been developed and implemented in Monte Carlo codes.

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2.1. Asymptotic model

The simplest model for the target velocity in an elastic scattering event is to assume that the target is at rest. Utilizing this zero-velocity target assumption is equivalent to modeling elastic scattering with the well known asymptotic kernel for isotropic scattering in the center of mass system (Duderstadt and Hamilton, 1976),

$$P(E \to E') = \begin{cases} \frac{1}{E(1-\alpha)} & \alpha E \leqslant E' \leqslant E \\ 0 & \text{otherwise} \end{cases}, \tag{1}$$

with E being the incident neutron energy, E' being the scattered neutron energy, and $\alpha \equiv (A-1)^2/(A+1)^2$, where A is the ratio of target mass to neutron mass. While this model is reasonable for scattering events with high incident neutron energies, it does not accurately capture the effects of target motion on thermal scattering kernels. Also, it has been shown that the asymptotic model, which does not permit upscattering into resonances, can dramatically misrepresent epithermal scattering kernels for resonant target nuclei (Ouisloumen and Sanchez, 1991). The misrepresentation manifests itself as a reduction in resonance absorption. This reduction has been shown to artificially increase k_{eff} results by ~200 pcm for LWR configurations. Even greater errors are observed in simulations of high-temperature reactor systems (Lee et al., 2009).

2.2. Constant cross section model

In order to eliminate the asymptotic model's assumption of a target at rest and take into account the thermal motion of target nuclei when considering the kinematics of elastic scattering, the velocity of the target must be determined. The ideal gas model is widely used for the treatment of epithermal neutron scattering in Monte Carlo codes (Carter and Cashwell, 1975). In this model, the motion of target nuclei is assumed to be isotropic, with speeds characterized by the classical Maxwell–Boltzmann distribution (Cullen and Weisbin, 1976). This distribution for target speed, v_t, in an ideal gas at temperature T is given by

$$M(T, v_t) = \frac{4}{\sqrt{\pi}}\beta^3 v_t^2 e^{-\beta^2 v_t^2}; \quad \beta \equiv \sqrt{\frac{Am_n}{2kT}}. \tag{2}$$

Here, k is the Boltzmann constant and m_n is the mass of a neutron.

The convolution of the Maxwell–Boltzmann distribution with the product of the relative speed between the neutron and target, v_{rel}, and the 0 K elastic scattering cross section yields an expression for the effective, reaction rate-preserving, Doppler broadened scattering cross section (Cullen and Weisbin, 1976),

$$\sigma_s(T, v_n) = \frac{1}{2v_n}\iint v_{rel}\sigma_s(0, v_{rel})M(T, v_t)dv_t d\mu, \tag{3}$$

in which v_n is the neutron speed. The relative speed is given by

$$v_{rel} = |\vec{v}_n - \vec{v}_t| = \sqrt{v_n^2 + v_t^2 - 2\mu v_n v_t}, \tag{4}$$

with μ being the cosine of the angle between the initial neutron and target direction vectors.

The Doppler broadened cross section can be recast as a joint probability density function (PDF),

$$P(v_t, \mu|v_n) = \frac{v_{rel}\sigma_s(0, v_{rel})M(T, v_t)}{2v_n\sigma_s(T, v_n)}, \tag{5}$$

for the correlated μ and v_t variables. The correlation of μ and v_t means that Eq. (5) cannot be sampled directly by sampling the PDFs of μ and v_t independently (Rothenstein, 1996).

By assuming that the 0 K scattering cross section of the target varies negligibly over the range of practically attainable v_{rel} values, the integral over μ in Eq. (3) can be evaluated analytically (Carter and Cashwell, 1975), enabling use of the sampling procedure outlined below. With the assumption of a constant cross section, the PDF is described by

$$P_{\text{CXS}}(v_t, \mu|v_n) \propto v_{rel}M(T, v_t). \tag{6}$$

The constant cross section approximation (CXS) is central to the target velocity sampling algorithm detailed by Gelbard (1979). This algorithm, in slightly varying forms, has long been the standard method for treating epithermal elastic scattering in Monte Carlo codes such as MCNP (X-5 Monte Carlo Team, 2008), MC21 (Sutton et al., 2007), and OpenMC (Romano and Forget, 2013). The approximation has been justified with the reasoning that the scattering cross sections of light nuclei are typically slowly varying in energy, and that heavy nuclei, whose scattering cross sections can vary sharply in energy, contribute so little to neutron moderation through elastic scattering that the effects of the approximation are negligible (X-5 Monte Carlo Team, 2008).

The sampling of Eq. (6) can be simplified with the inclusion of canceling $v_n + v_t$ terms which allow the distribution to be rewritten as

$$P_{\text{CXS}}(v_t, \mu|v_n) = C_{\text{CXS}}\frac{v_{rel}}{v_n + v_t}[v_n v_t^2 e^{-\beta^2 v_t^2} + v_t^3 e^{-\beta^2 v_t^2}]; \quad C_{\text{CXS}} = \frac{2\beta^3}{v_n\sqrt{\pi}}. \tag{7}$$

Having no dependence on target velocity, C_{CXS} is simply a normalization constant. Then, μ can be sampled uniformly and v_t can be obtained by sampling the distribution given by the bracketed terms in Eq. (7). The sampled target velocity specified by μ and v_t is then accepted with a probability equal to the ratio

$$R_{\text{CXS}} = \frac{v_{rel}}{v_n + v_t}. \tag{8}$$

2.3. Energy dependent cross section model

The CXS implementation of the ideal gas model addresses the inadequacy of the asymptotic model insofar as it assigns, through the procedure outlined in the previous section, a velocity to target nuclei. However, in the target velocity sampling procedure, the energy dependence of cross sections is neglected. It was shown analytically by Ouisloumen and Sanchez (1991) that, in the epithermal region, the strong energy dependence of resonant nuclei scattering cross sections can result in scattering kernels that are highly distorted from those given by the asymptotic model. The CXS ideal gas model cannot accurately calculate epithermal resonance scattering kernels because it neglects the scattering cross section energy dependence that is largely responsible for the distortion of resonant nuclei scattering kernels from an asymptotic shape. There exist multiple methods for correctly incorporating the effects of energy dependent scattering cross sections in epithermal scattering treatments.

2.3.1. Scattering law tables

Typically, $S(\alpha, \beta)$ scattering law tables are used to specify secondary energy and angular distributions for neutron scattering in the thermal region, where chemical binding effects may be significant. The capability to generate tables for nuclei with energy dependent cross sections was introduced into the NJOY Nuclear Data Processing System (Macfarlane and Muir, 1994) by Rothenstein (2004). The use of $S(\alpha, \beta)$ tables in modeling scattering from resonant nuclei, demonstrated by Dagan (2005), forgoes the sampling of a target velocity and, in doing so, avoids the problems