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An improved target velocity sampling algorithm for free gas elastic scattering

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ABSTRACT

We present an improved algorithm for sampling the target velocity when simulating elastic scattering in a Monte Carlo neutron transport code that correctly accounts for the energy dependence of the scattering cross section. The algorithm samples the relative velocity directly, thereby avoiding a potentially inefficient rejection step based on the ratio of cross sections. We have shown that this algorithm requires only one rejection step, whereas other methods of similar accuracy require two rejection steps. The method was verified against stochastic and deterministic reference results for upscattering percentages in ^{238}U. Simulations of a light water reactor pin cell problem demonstrate that using this algorithm results in a 3% or less penalty in performance when compared with an approximate method that is used in most production Monte Carlo codes.

1. Introduction

At sufficiently high incident neutron energies, the thermal motion of target nuclei with which neutrons collide can be safely assumed to be zero, implying that the double-differential scattering cross section is independent of the temperature of the material. At epithermal energies and below, however, it is important to account for the effect of target thermal motion on both the integrated cross section and the differential scattering cross section. The effect can be quantified by writing the reaction rate as a function of the target velocity:

$$v_r \sigma(v_r) M(T, \mathbf{V}), \tag{1}$$

where $\mathbf{V}$ is the target velocity, $v_r = |\mathbf{v} - \mathbf{V}|$, $\mathbf{v}$ is the velocity of the incident neutron in the laboratory system, T is the temperature of the material, $\sigma(v_r)$ is the 0 K cross section at relative velocity v_r, and $M(T, \mathbf{V})$ is the distribution of target velocities at temperature T. If one integrates Eq. (1) over all possible target velocities, the Doppler broadened reaction rate is found. One can then construct a multivariate probability distribution for $\mathbf{V}$ by dividing by this integral.

$$f(\mathbf{V}) = \frac{v_r \sigma(v_r) M(T, \mathbf{V})}{\int d\mathbf{V}\ v_r \sigma(v_r) M(T, \mathbf{V})} \tag{2}$$

Let us define C to be the inverse of the denominator of Eq. (2) so that

$$f(\mathbf{V}) = C v_r \sigma(v_r) M(T, \mathbf{V}). \tag{3}$$

The distribution in Eq. (3) represents the distribution of target velocities, $M(T, \mathbf{V})$, weighted by their expected contribution to the reaction rate.

Several assumptions are often made in order to simplify Eq. (3) into a form that can be sampled. The most common assumption is that the distribution of target velocities is an isotropic Maxwell–Boltzmann distribution for a monatomic ideal gas. This allows one to separately treat the magnitude and direction of the target velocity:

$$f(V, \mu, \varphi) = C v_r \sigma(v_r) M(T, V) f'(\mu) f''(\varphi), \tag{4}$$

where $V = |\mathbf{V}|$, $vV\mu = \mathbf{v} \cdot \mathbf{V}$, $v = |\mathbf{v}|$, and φ is the azimuthal angle. The Maxwell–Boltzmann distribution for the target speed is defined as

$$M(T, V) = \frac{4}{\sqrt{\pi}} \beta^3 V^2 e^{-\beta^2 V^3}, \tag{5}$$

where

$$\beta = \sqrt{\frac{m}{2kT}}, \tag{6}$$

m is the mass of the target nuclide, and k is Boltzmann's constant. $f'(\mu)$ is a uniform distribution over the interval $[-1, 1]$,

$$f'(\mu) = \frac{H(\mu + 1) - H(\mu - 1)}{2}, \tag{7}$$

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where H is the Heaviside step function, and $f''(\varphi)$ is a uniform distribution over the interval $[0, 2\pi]$,

$$f''(\varphi) = \frac{H(\varphi) - H(\varphi - 2\pi)}{2\pi}. \tag{8}$$

Because φ can be sampled independently of $\mathbf{V}$ and μ, the problem is reduced to sampling the bivariate distribution in V and μ,

$$f(V, \mu) = C v_r \sigma(v_r) M(T, V) f'(\mu). \tag{9}$$

Even with the monatomic ideal gas assumption, one still has to account for the dependence of the cross section on the relative velocity in Eq. (9). Thus, a further assumption is often made that the cross section is constant over the range of plausible relative velocities. This leads to a probability distribution in V and μ that can readily be sampled. However, this assumption can lead to significant errors in both the differential scattering cross section (Ouisloumen and Sanchez, 1991) and the calculated eigenvalue (Lee et al., 2009).

Various methods have been proposed to account for the energy dependence of the cross section when sampling target velocities in Monte Carlo (MC) neutron transport simulations. A rejection method, commonly referred to as the Doppler broadening rejection correction (DBRC), was proposed by Rothenstein (1996) and later popularized by Becker et al. (2009). Other authors have suggested using $S(\alpha, \beta)$ tables (Dagan, 2005) and weight corrections (Mori and Nagaya, 2009). The DBRC method has become nearly ubiquitous in modern MC codes, having been implemented in TRIPOLI (Zoia et al., 2013), MC21 (Trumbull and Fieno, 2013), Serpent (Leppänen et al., 2015), SuperMC (Wu et al., 2015), RMC (Liu et al., 2016), and OpenMC (Walsh et al., 2014).

The DBRC method can lead to very low rejection efficiencies near resonances, however, thereby increasing the execution time of a simulation. For example, Trumbull and Fieno (2013) found a 14% decrease in the figure of merit when applying the DBRC method to a light water reactor (LWR) pin cell problem. To address this inefficiency, Walsh et al. (2014) developed an algorithm that relies on directly sampling the relative velocity and then rejecting it based on a function of the target velocity (rather than the other way around as in the DBRC method). The method was implemented in OpenMC where it demonstrated better computational efficiency than did the DBRC method. In the present work, we improve upon this algorithm. By changing variables to the target energy and relative energy, we are able to directly sample the relative and target velocities and perform a single rejection step on μ. This approach results in a simpler algorithm that has little runtime overhead compared with that of the standard method of assuming a constant cross section. In addition, to aid code developers who may want to implement this method, we explicitly consider implementation details that were not discussed by Walsh et al. (2014).

2. Target velocity sampling methods

Before describing the improved target velocity sampling method, we first consider how the existing methods are implemented in an MC code. We begin with a complete description of the traditional method whereby the cross section is assumed to be independent of the incident neutron energy, which we call the *constant cross section* (CXS) method.

2.1. Constant cross section

Substituting Eq. (5) into Eq. (9) results in

$$f(V, \mu) = \frac{4C}{\sqrt{\pi}} v_r \sigma(v_r) \beta^3 V^2 e^{-\beta^2 V^2} f'(\mu). \tag{10}$$

Assuming that the cross section is constant over all v_r further implies that

$$f(V, \mu) \approx \frac{4\sigma C}{\sqrt{\pi}} v_r \beta^3 V^2 e^{-\beta^2 V^2} f'(\mu). \tag{11}$$

While μ and V can be sampled from terms appearing in Eq. (11), the difficulty is that v_r depends on both V and μ and is unbounded. To get around this, we first introduce a lemma from the theory of nonuniform random variate generation (Devroye, 1986).

Lemma 1. *Any density function of the form $f(\mathbf{x}) = cg(\mathbf{x})\psi(\mathbf{x})$ where $g(\mathbf{x})$ is a density function and $\psi(\mathbf{x})$ is $[0, 1]$-valued can be sampled by drawing $\mathbf{x}'$ from $g(\mathbf{x})$ and accepting it with probability $\psi(\mathbf{x}')$*

One can deduce from geometric considerations that v_r cannot attain a value greater than $v + V$. Thus, multiplying and dividing Eq. (11) by $v + V$, we obtain

$$f(V, \mu) = \frac{4\sigma C}{\sqrt{\pi}} \frac{v_r}{v + V} \left(v\beta^3 V^2 e^{-\beta^2 V^2} + \beta^3 V^3 e^{-\beta^2 V^2} \right) f'(\mu). \tag{12}$$

Changing variables to $x = \beta V$, defining $y = \beta v$, normalizing the density function inside parentheses, and rearranging, one reaches the following expression:

$$f(x, \mu) = C_{\text{CXS}} \frac{\beta v_r}{x + y} \left[\left(\frac{\sqrt{\pi} y}{\sqrt{\pi} y + 2} \right) \frac{4}{\sqrt{\pi}} x^2 e^{-x^2} + \left(\frac{2}{\sqrt{\pi} y + 2} \right) 2x^3 e^{-x^2} \right] f'(\mu) \tag{13}$$

In Eq. (13), the term inside the brackets is a discrete mixture of two densities that can be easily sampled. Thus, the sampling algorithm for V and μ proceeds as follows. First, sample μ uniformly from $f'(\mu)$. Then, with probability $2/(\sqrt{\pi} y + 2)$ sample the distribution $2x^3 e^{-x^2}$. Otherwise, sample the distribution $4/\sqrt{\pi} x^2 e^{-x^2}$. Using Lemma 1, the resulting x and μ values are accepted with probability $\beta v_r / (x + y)$. If they are rejected, the process is repeated. A complete algorithm is shown in Algorithm 1. Note that each instance of ξ refers to a pseudorandom number drawn from a uniform distribution on $[0, 1)$.

Algorithm 1. Target velocity sampling algorithm assuming constant cross section

```
function SAMPLEVELOCITYCXS(v)
  y ← βv
  loop
    μ ← 2ξ1 − 1
    if ξ2 < 2/(√π y + 2) then
      z ← − log(ξ3 ξ4)
    else
      z ← − log ξ3 − cos²(π/2 ξ4) log ξ5
    end if
    x ← √z
    if ξ6 < (y² + z − 2xyμ)/(y + x) then
      V ← x/β
      return V, μ
    end if
  end loop
end function
```

2.2. Doppler broadening rejection correction

As noted earlier, assuming that the elastic scattering cross section is constant over energies close to that of the incident neutron is not reasonable when scattering resonances are present. To account for the shape of the cross section on the sampled distribution of target velocities, we return to Eq. (10) and proceed as we