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Analytic Sensitivity Coefficients for Bethe's Solution of the Neutron Slowing Down Equation

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ABSTRACT

Neutron slowing down theory is used to derive expressions for the sensitivity coefficients of the neutron collision density in a hydrogenous infinite medium with respect to the fixed source, scattering probability, and macroscopic nuclear cross sections. Analytic expressions for Bethe's solution of the neutron slowing down equation are derived for the constant cross section approximation with a point, uniform, and gamma lethargy spectrum. Analytic expressions for the corresponding sensitivity coefficients are derived and used to verify Monte Carlo neutron transport calculations.

Keywords: analytic benchmark, sensitivity coefficient, Hans Bethe, neutron slowing down theory

1. INTRODUCTION

In 1937, Hans Bethe wrote [1]

> The phenomena produced by slow neutrons have been of the greatest importance for the development of the modern theory of nuclear processes. They supply the most detailed information yet available on the energy levels of heavy nuclei.

The theory in question was developed by investigating the behavior of neutrons in hydrogen-containing substances such as water or paraffin, which are used to slow down neutrons in neutron-nucleus cross section measurement experiments. Bethe posed three main questions that needed to be resolved before the more fundamental questions pertaining to the resonance parameters of these primitive nuclear data evaluations could be addressed thoroughly, namely,

> (1) What is the energy distribution of the neutrons in a pure infinitely extended hydrogeneous substance?
>
> (2) What is the distribution of the neutrons in space, and how does it depend on the neutron energy?
>
> (3) How are the distributions affected if an absorbing substance is placed inside the hydrogeneous substance?

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Bethe addressed these problems using a simple theoretical framework for neutron slowing down theory, where he relied on experimentally determined constants, such as the mean free path of slow neutrons, to make predictions, evaluate the measured data, and update his hypotheses. This approach is identical to contemporary scientific discovery except now advanced numerical methods are used to make experimental predictions instead of the "reasonable theoretical assumptions" asserted by Bethe *et al.* at that time. Today, Bethe's solution of the neutron slowing down equation is still relevant as an analytic benchmark that can be used to verify advanced numerical transport calculations.

This paper reviews Bethe's solution of the neutron slowing down equation by way of Dawn's generalized exact solution [2], which addresses Bethe's first and third questions, and asks a fourth question:

> (4) How sensitive are these distributions to perturbations of the fixed neutron source, scattering probability, and macroscopic nuclear cross sections?

This question is relevant for the sensitivity analysis, uncertainty quantification, and data assimilation techniques that are developed for use in nuclear applications on modern-day super-computers. It is answered by deriving analytic expressions for the relevant sensitivity coefficients of Bethe's solution and using them to verify the numerical results of advanced Monte Carlo neutron transport methods.

2. MOTIVATION

This paper focuses on Bethe's original description of the neutron slowing down equation. Other works have generalized the neutron slowing down equation to include multiple non-hydrogenous fissionable isotopes [3], extended it to eigenvalue problems [4], and found the corresponding k-eigenvalue sensitivity coefficients [5]. In contrast, this work only intends to extend Bethe's original fixed-source results to include an analytic sensitivity analysis. This approach affords the neutron transport practitioner a simple set of elementary expressions that can easily be included in their verification benchmark test suite. To that end, Bethe's solution of the neutron slowing down equation is reviewed, and the results are used to derive general expressions for the corresponding sensitivity coefficients with respect to the fixed source, scattering probability, and macroscopic nuclear cross sections.

2.1. Review of Bethe's Solution

The neutron transport equation is used to predict the energy distribution of neutrons in a mono-atomic infinite medium, where the only relevant reactions are capture and scattering,

$$\Sigma_T(E)\phi(E) = Q(E) + \int_0^\infty \Sigma_S(E' \to E)\phi(E')dE'. \tag{1}$$

The variables in this equation are defined as follows:

$\Sigma_T(E) = \Sigma_C(E) + \Sigma_S(E)$ is the energy dependent total macroscopic cross section,
$\Sigma_C(E)$ is the energy dependent capture macroscopic cross section, i.e., no neutrons emitted,
$\Sigma_S(E' \to E)$ is the differential scattering macroscopic cross section, which becomes the energy dependent scattering macroscopic cross section, $\Sigma_S(E')$, when integrated over all outgoing neutron energies, E,
$\phi(E)$ is the energy dependent scalar neutron flux, and
$Q(E)$ is the energy dependent fixed source of neutrons in the system, which emits neutrons with a maximum energy of E_0.

Bethe considered this equation for neutrons with energies above 1 (electron)volt in a purely hydrogenous medium, i.e., s-wave scattering off protons. In these systems, a neutron of energy E' has equal probability of elastically scattering anywhere in the range $(0, E')$. It follows that the differential scattering macroscopic cross section in the transport equation is expressed only in terms of the incident neutron energy, E',

$$\Sigma_T(E)\phi(E) = Q(E) + \int_E^{E_0} \frac{\Sigma_S(E')}{E'}\phi(E')dE'. \tag{2}$$

A familiar form of this neutron slowing down equation is recovered by instead solving for the neutron collision density, $F(E) \equiv \Sigma_T(E)\phi(E)$,

$$F(E) = Q(E) + \int_E^{E_0} \frac{\gamma(E')}{E'}F(E')dE', \tag{3}$$

where Dawn's notation is used to define the scattering probability $\gamma(E) \equiv \Sigma_S(E)/\Sigma_T(E)$. This equation is re-cast in terms of the neutron lethargy,

$$u(E) \equiv \ln\left(\frac{E_0}{E}\right), \tag{4}$$

where $E_0 \geq E$, with the result that

$$F(u) = Q(u) + \int_0^u \gamma(u') \exp\left(u' - u\right) F(u')du'. \tag{5}$$

Bethe originally found the solution to this Volterra integral equation of the second kind for point sources. However, the generalized exact solution provided by Dawn is the motivating equation for deriving sensitivity coefficients in this paper. That solution is

$$F(u) = Q(u) + \int_0^u Q(u')\gamma(u') \exp\left\{\int_{u'}^u \left[\gamma(u'') - 1\right] du''\right\}du' \tag{6}$$

for continuous-lethargy cross sections, which reduces to

$$F(u) = Q(u) + \int_0^u Q(u')du' \tag{7}$$

for pure scattering problems ($\gamma = 1$) and

$$F(u) = Q(u) \tag{8}$$

for pure capture problems ($\gamma = 0$).

2.2. Derivation of the Sensitivity Coefficients

A sensitivity coefficient describes the fractional change in a system response, which in this work is the neutron collision density, $F(u)$, due to a fractional change in a system parameter, denoted here by the generic variable α,

$$S_{F(u),\alpha} = \frac{\partial F(u)/F(u)}{\partial \alpha/\alpha}. \tag{9}$$

A transformation of the neutron collision density from lethargy space to energy space does not change the absolute number of neutrons colliding in the phase space volume element. To accommodate this transformation, it is required that

$$|F(u)du| = |F(E)dE| \implies F(u) = F(E)\left|\frac{dE}{du}\right| \implies F(u) = EF(E), \tag{10}$$

which means that the sensitivity coefficient remains the same in either variable,

$$S_{F(u),\alpha} = \frac{\partial F(u)/F(u)}{\partial\alpha/\alpha} = \frac{\partial\left[EF(E)\right]/\left[EF(E)\right]}{\partial\alpha/\alpha} = \frac{\partial F(E)/F(E)}{\partial\alpha/\alpha} = S_{F(E),\alpha}. \tag{11}$$

In the following subsections, general expressions for the fixed source, scattering probability, and cross section sensitivities are derived using Bethe's solution of the neutron slowing down equation. These expressions are then used to derive expressions for a few analytically tractable test cases and the results are used to verify two numerical methods.

2.2.1. Fixed-Source Sensitivities

Suppose that the fixed source is parameterized by an arbitrary set of variables $\alpha \in \{a, b, c, \ldots\}$, which are interpreted as the values of a histogram or the parameters of a continuous distribution. The sensitivity of the neutron collision density with respect to any of these parameters is obtained as

$$S_{F(u),\alpha} = \frac{\alpha}{F(u)}\left[\frac{\partial Q(u)}{\partial\alpha} + \int_0^u \frac{\partial Q(u')}{\partial\alpha}\gamma(u')\exp\left\{\int_{u'}^u\left[\gamma(u'') - 1\right]du''\right\}du'\right]. \tag{12}$$

For pure scattering problems ($\gamma = 1$) this reduces to

$$S_{F(u),\alpha} = \frac{\alpha}{F(u)}\left[\frac{\partial Q(u)}{\partial\alpha} + \int_0^u \frac{\partial Q(u')}{\partial\alpha}du'\right], \tag{13}$$

and for pure capture problems ($\gamma = 0$) this reduces to

$$S_{F(u),\alpha} = \frac{\alpha}{F(u)}\frac{\partial Q(u)}{\partial\alpha} = \frac{\alpha}{Q(u)}\frac{\partial Q(u)}{\partial\alpha} = S_{Q(u),\alpha}. \tag{14}$$

2.2.2. Scattering Probability and Cross Section Sensitivities

Bethe's solution of the neutron collision density is parameterized by three macroscopic cross sections through the scattering probability, $\gamma(u) = \Sigma_S(u)/\Sigma_T(u)$, where $\Sigma_T(u) = \Sigma_C(u) + \Sigma_S(u)$. The scattering probability and cross section sensitivity coefficients are found by taking the relative partial derivative of the neutron collision density with respect to any one of these parameters, $\alpha \in \{\gamma, \Sigma_C, \Sigma_S, \Sigma_T\}$,

$$S_{F(u),\alpha} = \frac{\alpha}{F(u)}\int_0^u Q(u')\left[\frac{\partial\gamma(u')}{\partial\alpha} + \gamma(u')\int_{u'}^u\frac{\partial\gamma(u'')}{\partial\alpha}du''\right]\exp\left\{\int_{u'}^u\left[\gamma(u'') - 1\right]du''\right\}du', \tag{15}$$

where the derivative of the scattering probability is found through application of the quotient rule from differential calculus,

$$\frac{\partial\gamma(u)}{\partial\alpha} = \frac{\Sigma_T(u)\left[\partial\Sigma_S(u)/\partial\alpha\right] - \Sigma_S(u)\left[\partial\Sigma_T(u)/\partial\alpha\right]}{\Sigma_T(u)^2}. \tag{16}$$

In the special case that the scattering probability is a constant function of lethargy, its relative sensitivity coefficient with respect to the macroscopic cross sections reduces to

$$S_{\gamma,\Sigma_C} = \gamma - 1 \tag{17}$$

for capture,

$$S_{\gamma,\Sigma_S} = 1 - \gamma \tag{18}$$

for scattering, and

$$S_{\gamma,\Sigma_T} = 0 \tag{19}$$

for the total macroscopic cross section. These expressions are used to transform the scattering probability sensitivity coefficient into any one of the cross section sensitivity coefficients, Σ_X,

$$S_{F(u),\Sigma_X} = S_{F(u),\gamma} S_{\gamma,\Sigma_X}. \tag{20}$$

3. ANALYTIC RESULTS

The general expressions derived above are applied to a few analytically tractable test cases in which the constant cross section approximation is applied to systems with a point source, uniform source, and gamma lethargy spectrum. The rationale for choosing these particular fixed sources goes as follows: Bethe originally examined point sources; the uniform source exhibits interesting limiting behavior at the source boundary and can be made to be a point source; and the gamma lethargy spectrum represents a wide range of neutron source physics.

3.1. Point Source

A point source is defined as Dirac's delta function centered around zero lethargy with source strength $Q > 0$,

$$Q(u) = Q\delta(u). \tag{21}$$

The neutron collision density for the constant cross section approximation with a point source is

$$F(u) = Q\delta(u) + Q\gamma \exp\left[(\gamma - 1)u\right], \tag{22}$$

which is identical to Bethe's original solution for $u > 0$,

$$F(u^+) = Q\gamma \exp\left[(\gamma - 1)u\right]. \tag{23}$$

The scattering probability sensitivity coefficient is

$$S_{F(u^+),\gamma} = 1 + \gamma u, \tag{24}$$

and the cross section sensitivity coefficients are

$$S_{F(u^+),\Sigma_C} = (1 + \gamma u)(\gamma - 1) \tag{25}$$

for capture,

$$S_{F(u^+),\Sigma_S} = (1 + \gamma u)(1 - \gamma) \tag{26}$$

for scattering, and

$$S_{F(u^+),\Sigma_T} = 0 \tag{27}$$

for the total macroscopic cross section.

These expressions represent the sensitivity of the neutron collision density to a global perturbation of the scattering probability and macroscopic cross sections in the incoming neutron lethargy variable. However, the local sensitivity coefficients are often what is required to perform sensitivity and uncertainty analysis of a problem. Analytic expressions for these local sensitivity coefficients are found by restricting the application of the partial derivative to a specific lethargy range of interest,

$$I_{(a,b)}(u) \frac{\partial}{\partial \alpha} \left\{\cdot\right\}, \tag{28}$$

where the indicator function $I_{(a,b)}(u)$ is 1 if $u \in (a, b)$ for $0 \leq a \leq b$ and 0 otherwise. Substituting this into Equation 15 for each partial derivative and making the constant cross section and point source approximations yields

$$S_{F(u),\gamma} = I_{\{0\}}(a) + \gamma \left[\min(u, b) - \max(a, 0)\right] I_{(a,\infty)}(u) \tag{29}$$

for the scattering probability sensitivity coefficient. The global sensitivity coefficient is recovered by letting $a = 0$ and $b \to \infty$, and the point sensitivity is found by letting $a = b$,

$$S_{F(u),\gamma} = I_{\{0\}}(a), \tag{30}$$

which means that the neutron collision density is not sensitive to perturbations of the scattering probability at a single point unless that point coincides with the fixed source.

3.2. Uniform Source

A uniform source is defined as a constant over the lethargy range of interest with source strength $Q > 0$ and zero everywhere else,

$$Q(u) = \frac{Q}{u_{\max}} \begin{cases} 1 & 0 \leq u \leq u_{\max} \\ 0 & u > u_{\max} \end{cases}. \tag{31}$$

The neutron collision density for the constant cross section approximation with a uniform source is

$$F(u) = \frac{Q}{u_{\max}} \frac{\gamma}{\gamma - 1} \begin{cases} \exp\left[(\gamma - 1) u\right] - 1/\gamma & 0 \leq u \leq u_{\max} \\ \left(1 - \exp\left[-(\gamma - 1) u_{\max}\right]\right) \exp\left[(\gamma - 1) u\right] & u > u_{\max} \end{cases}, \tag{32}$$

and the global scattering probability sensitivity coefficient is

$$S_{F(u),\gamma} = \frac{\left(\gamma (\gamma - 1) u - 1\right) \exp\left[(\gamma - 1) u\right] + 1}{(\gamma - 1)\left(\exp\left[(\gamma - 1) u\right] - 1/\gamma\right)} \tag{33}$$

for $0 \leq u \leq u_{\max}$ and

$$S_{F(u),\gamma} = \frac{\gamma (\gamma - 1) u - 1 + \left(\gamma (\gamma - 1)(u_{\max} - u) + 1\right) \exp\left[-(\gamma - 1) u_{\max}\right]}{(\gamma - 1)\left(1 - \exp\left[-(\gamma - 1) u_{\max}\right]\right)} \tag{34}$$

for $u > u_{\max}$.

The Maclaurin series of $\exp\left[-(\gamma - 1) u_{\max}\right]$ with respect to $u_{\max}$ is truncated to $1 - (\gamma - 1) u_{\max}$ and used to simplify these expressions in the case that $u_{\max} \to 0^+$, i.e., the fixed source approaches a delta function, with the result that the neutron collision density and sensitivity coefficients approach the point source expressions.

3.3. Gamma Lethargy Spectrum

A wide variety of neutron slowing down problems can be examined if the fixed source is chosen to be

$$Q(u) = Q \frac{(bE_0)^a}{\Gamma(a)} \exp\left[-\left(au + bE_0 \exp(-u)\right)\right], \quad u \in (-\infty, \infty), \quad a, b \in \mathbb{R}_{>0}, \tag{35}$$

where $Q > 0$ is the source strength and $\Gamma(x)$ is the complete gamma function. In neutron energy space, this transforms to the well-known gamma distribution,

$$Q(E) = Q \frac{b^a}{\Gamma(a)} E^{a-1} \exp(-bE), \quad E \in (0, \infty), \quad a, b \in \mathbb{R}_{>0}, \tag{36}$$

which is an attractive model for real-world neutron sources. For example, when the shape parameter, a, is 1, 3/2, and 2 the related distributions in energy space are the exponential, Maxwell-Boltzmann, and evaporation energy distributions, respectively, and for large a the gamma distribution converges to a normal distribution with mean $\mu = a/b$ and variance $\sigma^2 = a/b^2$. This makes the gamma lethargy spectrum an excellent candidate for exploring neutron slowing down theory.

For pure scattering problems ($\gamma = 1$) with a fixed source defined by a gamma distribution the neutron collision density is

$$F(u) = \frac{Q}{\Gamma(a)} \left[(bE_0)^a \exp\left[-\left(au + bE_0 \exp(-u)\right)\right] + \Gamma\left(a, bE_0 \exp(-u)\right) - \Gamma\left(a, bE_0\right) \right], \tag{37}$$

where $\Gamma(x, y)$ is the upper incomplete gamma function and the sensitivity coefficient with respect to the rate parameter, b, is

$$S_{F(u),b} = \frac{\left(a - 1 - bE_0 \exp(-u)\right) \exp\left[-\left(au + bE_0 \exp(-u)\right)\right] + \exp(-bE_0)}{\exp\left[-\left(au + bE_0 \exp(-u)\right)\right] + \left[\Gamma\left(a, bE_0 \exp(-u)\right) - \Gamma\left(a, bE_0\right)\right] / (bE_0)^a}. \tag{38}$$

For pure capture problems ($\gamma = 0$) the neutron collision density is

$$F(u) = \frac{Q}{\Gamma(a)} (bE_0)^a \exp\left[-\left(au + bE_0 \exp(-u)\right)\right], \tag{39}$$

the sensitivity coefficient with respect to the rate parameter, b, is

$$S_{F(u),b} = a - bE_0 \exp(-u), \tag{40}$$

and the sensitivity coefficient with respect to the shape parameter, a, is

$$S_{F(u),a} = a \left(\ln(bE_0) - u - \Psi(a)\right), \tag{41}$$

where $\Psi(x)$ is the digamma function.

Equations 40 and 41 represent the sensitivity of the fixed source, $Q(u)$, to the rate and shape parameters, respectively, and the sensitivity to the shape parameter more specifically represents the sensitivity of the neutron collision density to the model underlying the fixed source, e.g., when $a = 3/2$ this represents the sensitivity of the neutron collision density to the Maxwell-Boltzmann distribution. Although these expressions seem to be relevant only to pure capture solutions of the neutron transport equation, it is demonstrated in the next section that they are used to find the sensitivity of any integrated reaction rate response to the fixed source of any neutron transport problem.

4. MONTE CARLO METHODS AND RESULTS

This section presents numerical results from the MCNP6.3 [6] software for the neutron collision density and cross section sensitivity coefficients for the problems described above. The MCNP® radiation transport code does not currently support sensitivity calculations with respect to the parameters of a continuous fixed source. It has been shown that source sensitivity calculations with respect to a histogram representation of a fixed source can be performed in a post-processing routine of Monte Carlo results [7], but application of this method to continuous fixed-source problems would be an approximation of the desired results. Individual Monte Carlo histories are required to estimate the exact solution of continuous fixed-source sensitivity calculations. This can also be achieved in a post-processing routine if the individual histories are recorded by the program, but such an approach may be prohibitively expensive. A Monte Carlo method for making these calculations on-the-fly is presented and verified against the analytic fixed-source sensitivity coefficients using a toy code.

4.1. Fixed-Source Sensitivity Calculations via the Green's Function Method

The Monte Carlo transport technique can be used to calculate continuous-lethargy fixed-source sensitivity coefficients. This method takes advantage of the fact that Monte Carlo transport implicitly samples from a Green's function of the neutron transport operator,

$$\mathcal{L}\phi(u) = Q(u), \tag{42}$$

where for this specific problem

$$\mathcal{L}\phi(u) \equiv \Sigma_T(u)\phi(u) - \int_0^u \Sigma_S(u') \exp(u' - u)\, \phi(u')du'. \tag{43}$$

In Monte Carlo transport, the continuous-lethargy neutron collision density is approximated by a normalized integral,

$$F_i = \frac{1}{u_{i+1} - u_i} \int_{u_i}^{u_{i+1}} \Sigma_T(u)\phi(u)du, \tag{44}$$

where integration is performed over the i-th lethargy range (u_i, u_{i+1}). The sensitivity of the integrated neutron collision density with respect to a fixed-source parameter, α, is found by taking the partial derivative of this expression with respect to α,

$$\frac{\partial F_i}{\partial \alpha} = \frac{1}{u_{i+1} - u_i} \int_{u_i}^{u_{i+1}} \Sigma_T(u) \frac{\partial \phi(u)}{\partial \alpha} du. \tag{45}$$

Evaluating this expression requires knowledge of how the lethargy-dependent neutron flux, $\phi(u)$, instantaneously changes with respect to the source parameter, α. This is found by differentiating the neutron transport equation with respect to α,

$$\mathcal{L}\frac{\partial \phi(u)}{\partial \alpha} = \frac{\partial Q(u)}{\partial \alpha}. \tag{46}$$

The neutron transport operator, $\mathcal{L}$, is formally inverted via the Green's function method,

$$\frac{\partial \phi(u)}{\partial \alpha} = \mathcal{L}^{-1}\frac{\partial Q(u)}{\partial \alpha} = \int_0^\infty \frac{\partial Q(u')}{\partial \alpha} G(u' \to u)du', \tag{47}$$

where $G(u' \to u)$ is the Green's function of the neutron transport operator, $\mathcal{L}$, which is interpreted as the neutron flux at u from a unit point source centered around u'. Inserting this expression into Equation 45 yields

$$\frac{\partial F_i}{\partial \alpha} = \frac{1}{u_{i+1} - u_i} \int_{u_i}^{u_{i+1}} \int_0^\infty \frac{\partial Q(u')}{\partial \alpha} G(u' \to u)\Sigma_T(u)du'du, \tag{48}$$

which is normalized to find an expression for the relative sensitivity coefficient,

$$S_{F_i,\alpha} = \frac{1}{F_i\,(u_{i+1} - u_i)} \int_{u_i}^{u_{i+1}} \int_0^\infty Q(u') \frac{\partial Q(u')/Q(u')}{\partial \alpha/\alpha} G(u' \to u)\Sigma_T(u)du'du, \tag{49}$$

where a factor of $Q(u')/Q(u')$ is introduced into the integrand to normalize the sensitivity coefficient of the fixed source with respect to α.

In Monte Carlo transport, continuous-lethargy fixed-source sensitivity calculations are made by multiplying the zeroth statistical moment of the neutron collision density tally by the sensitivity of the fixed source with respect to the source parameter of interest evaluated at the source lethargy, which is done at the end of the neutron's history. The result is normalized by the estimated neutron collision density at the end of the simulation if a relative sensitivity coefficient is desired. This method was implemented in a toy Monte Carlo code and verified against the analytic results to demonstrate that it works as expected. Algorithm 1 outlines the method and can be used as a template to reproduce the results for Bethe's solution of the neutron slowing down equation with a gamma lethargy spectrum and $a = 1$, which coincides with an exponential distribution in neutron energy space. This method can be extended to any fixed-source neutron transport problem for any integrated reaction rate response and any order sensitivity coefficient that is desired.

Monte Carlo estimates of the neutron collision density and rate sensitivity profile are calculated for the pure scattering case ($\gamma = 1$) and verified against the analytic results for the gamma lethargy spectrum, where $a = 1$, $b = 1/1.2895$ [1/MeV], and $E_0 = 20$ [MeV]. Figure 1 depicts the results and demonstrates excellent agreement between the numerical method and theory. In a pure scattering system, neutrons slow down and asymptotically approach a constant neutron collision density at high lethargy values. Increasing the rate parameter of the exponential distribution increases the probability that a low energy neutron will be born, and the sensitivity profile reflects this behavior as the coefficients are increasingly negative towards zero lethargy.

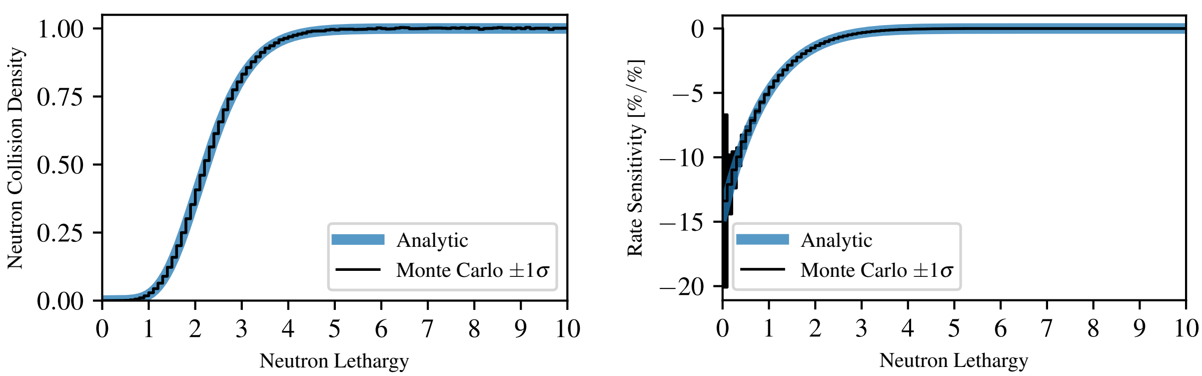

Figure 1. Verification of the Monte Carlo calculated neutron collision density and rate sensitivity profile for Bethe's pure scattering solution ($\gamma = 1$) of the neutron slowing down equation with a gamma lethargy spectrum ($a = 1$, $b = 1/1.2895$ [1/MeV], and $E_0 = 20$ [MeV])

Monte Carlo estimates of the shape and rate sensitivity profiles are calculated for the pure capture case ($\gamma = 0$) and verified against the analytic results for the gamma lethargy spectrum, where $a = 1$, $b = 1/1.2895$ [1/MeV], and $E_0 = 20$ [MeV]. Figure 2 depicts the results and demonstrates excellent agreement between the numerical method and theory. In a pure capture system, the neutron collision density is identical in shape to the fixed-source distribution. Increasing the shape parameter shifts the underlying distribution from an exponential source towards a Maxwell fission energy spectrum, which results in an increase of neutrons at higher birth energies. This is reflected in the linear behavior of the shape sensitivity profile. The interpretation of the rate sensitivity profile is consistent with the pure scattering case.

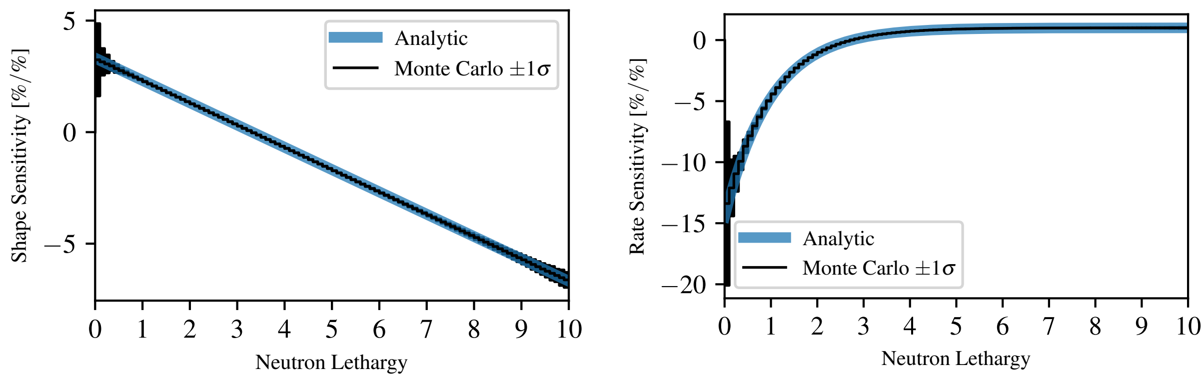

Figure 2. Verification of the Monte Carlo calculated shape and rate sensitivity profiles for Bethe's pure capture solution ($\gamma = 0$**) of the neutron slowing down equation with a gamma lethargy spectrum (**$a = 1$**,** $b = 1/1.2895$ **[1/MeV], and** $E_0 = 20$ **[MeV])**

4.2. Cross Section Sensitivity Calculations via the Differential Operator Method

Monte Carlo estimates of the neutron collision density and cross section sensitivity coefficients are calculated using the MCNP6.3 software and verified against the analytic results for the point and uniform source. The track-length (`F4`) tally and perturbation (`PERT`) cards are used in conjunction with the prescription described in [8] for first-order sensitivity analysis with exact uncertainty via the differential operator method. The results depicted in Figures 3 and 4 indicate excellent agreement between the MCNP6.3 software results and theory.

The neutron collision density for a point source in an infinite hydrogenous medium with some capture ($\gamma = 0.5$) decays exponentially in lethargy space, as shown in Figure 3. The sensitivity profile indicates that locally increasing the scattering cross section in the lethargy range $4 \leq u \leq 6$ results in zero sensitivity followed by a linear ramp to a constant value. The capture sensitivity is the negative of this result, and the total sensitivity is zero.

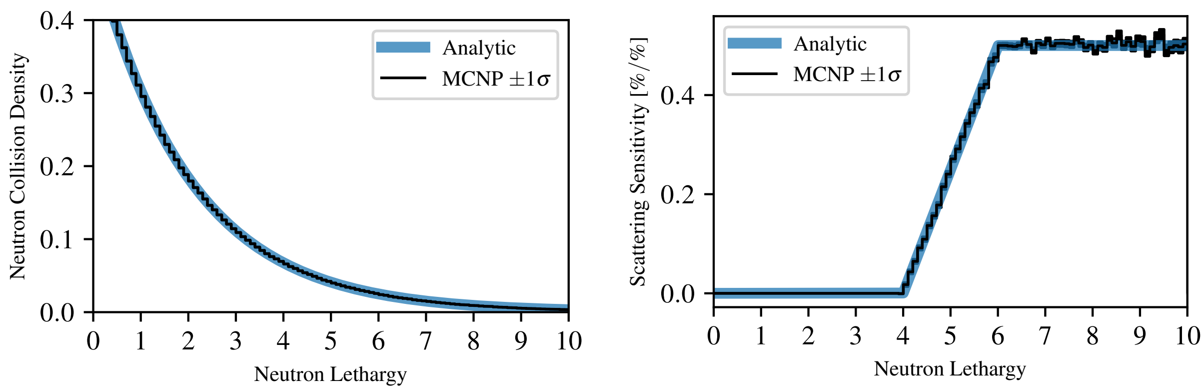

Figure 3. Verification of the MCNP6.3 [6] software calculated neutron collision density and local ($4 \leq u \leq 6$**) scattering sensitivity profile for Bethe's solution (**$\gamma = 0.5$**) of the neutron slowing down equation with a point source**

The neutron collision density for a uniform source ($u_{\max} = 5$) in a medium with some capture ($\gamma = 0.5$) increases within the source range, is discontinuous at the source boundary, and decays exponentially for all higher lethargy values, as shown in Figure 4. The sensitivity profile indicates that globally increasing the scattering cross section results in a slow increase towards the discontinuity at the source boundary, which is followed by a linear ramp for all higher lethargy values. The capture sensitivity is the negative of this result, and the total sensitivity is zero.

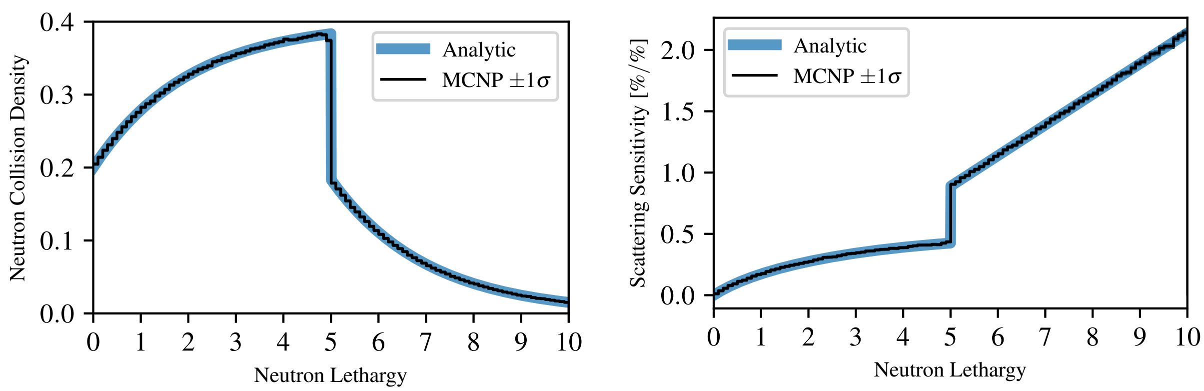

Figure 4. Verification of the MCNP6.3 [6] software calculated neutron collision density and global scattering sensitivity profile for Bethe's solution ($\gamma = 0.5$) of the neutron slowing down equation with a uniform source ($u_{\max} = 5$)

5. CONCLUSIONS

This work presents an extension of Bethe's solution of the neutron slowing down equation to all of the relevant sensitivity coefficients available for the problem. Dawn's notation and generalized exact solution is used to motivate general expressions for the sensitivity coefficients of the neutron collision density with respect to the fixed source, scattering probability, and macroscopic nuclear cross sections. It is shown that relative sensitivity coefficients are the same in either the neutron energy or lethargy variables, which allows the expressions developed in this work to be used as a benchmark for continuous-energy neutron transport calculations. A few analytically tractable test cases are considered and exact expressions for the neutron collision density and sensitivity coefficients are derived for a point source, uniform source, and gamma lethargy spectrum in conjunction with the constant cross section approximation. The analytic results are used to verify the numerical results of the radiation transport code MCNP6.3, and a method for extending Monte Carlo sensitivity calculations to continuous fixed-source problems is presented and verified. This work can be used as an analytic benchmark to verify the results of any fixed-source neutron transport code. In the future, the work presented here will be extended to include Dawn's generalized exact solution for neutron slowing down problems in any non-hydrogenous mono-atomic infinite medium.

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APPENDIX A. CONTINUOUS-LETHARGY FIXED-SOURCE SENSITIVITY CALCULATIONS IN MONTE CARLO NEUTRON TRANSPORT

Algorithm 1 Monte Carlo transport for Bethe's solution of the neutron slowing down equation with a gamma lethargy spectrum and $a = 1$

```
N ← number of particle histories
mesh max ← maximum lethargy bin boundary
M ← number of lethargy bins
Δu ← mesh max / M
S[1 to M][1 to 2] ← 0                         ▷ Initialize a M × 2 sensitivity vector
F[1 to M][1 to 3] ← 0                         ▷ Initialize a M × 3 collision density vector
for n ← 1 to N do                             ▷ Loop over N particle histories
    w ← 1                                     ▷ Initialize particle weight
    r ← random number ∈ (0, 1)
    u ← −ln(−ln(r)/b/E_0)                     ▷ Sample from the source distribution
    u_0 ← u                                   ▷ Store initial lethargy for sensitivity calculation
    while True do                             ▷ Loop over all particle collisions
        r ← random number ∈ (0, 1)
        d ← −ln(r)/Σ_T(u)                     ▷ Sample a distance to collision
        score ← Σ_T(u) · d · w                ▷ Calculate the track-length collision density score
        m ← ⌊u/Δu⌋                            ▷ Mesh index for u
        F[m][1] ← F[m][1]+ score              ▷ Zeroth moment
        w ← w · Σ_S(u)/Σ_T(u)                 ▷ Implicit capture
        r ← random number ∈ (0, 1)
        u ← u − ln(r)                         ▷ Calculate the new lethargy after scattering
        if u ≥ mesh max then
            break                             ▷ Exit the collision loop if the lethargy exceeds the mesh max
        end if
    end while
    multiplier ← ln(b · E_0) − u_0 − Ψ(1)     ▷ Calculate the analytic shape sensitivity, or
    multiplier ← 1 − b · E_0 · exp(−u_0)      ▷ Calculate the analytic rate sensitivity
    for m ← 1 to M do                         ▷ Loop over all mesh bins
        S[m][1] ← S[m][1]+ multiplier ·F[m][1]            ▷ First moment
        S[m][2] ← S[m][2] + (multiplier ·F[m][1])^2       ▷ Second moment
        F[m][2] ← F[m][2] + F[m][1]                       ▷ First moment
        F[m][3] ← F[m][3] + F[m][1]^2                     ▷ Second moment
        F[m][1] ← 0                                       ▷ Reset zeroth moment
    end for
end for
for m ← 1 to M do                             ▷ Loop over all mesh bins
    S[m][2] ← S[m][2]/(S[m][1])^2 − 1/N       ▷ Relative variance
    S[m][1] ← S[m][1]/F[m][2]                 ▷ Sensitivity coefficient
    S[m][2] ← |S[m][1]| sqrt(S[m][2])         ▷ Absolute standard deviation
    F[m][3] ← F[m][3]/(F[m][2])^2 − 1/N       ▷ Relative variance
    F[m][2] ← F[m][2]/Δu/N                    ▷ Collision density
    F[m][3] ← F[m][2] sqrt(F[m][3])           ▷ Absolute standard deviation
end for
```