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VERITAS

Visual Explorer for Real vs. Idealized neutron Transport and Analytic Solutions

DEVELOPER MANUAL

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1. Introduction

The VERITAS (Visual Explorer for Real vs. Idealized neutron Transport and Analytic Solutions) simulator is a high-fidelity computational tool designed to model the process of neutron moderation across a variety of media and environmental conditions. By leveraging the OpenMC Monte Carlo particle transport code, VERITAS provides users with an intuitive yet rigorous platform for visualizing the stochastic nature of neutron interactions.

The software is primarily intended as an educational resource for students learning nuclear physics fundamentals, as well as a versatile tool for entry-level research and preliminary design studies.

The simulator is documented in three manuals:

- User Manual – Describing the operation of the simulator from the user's perspective.
- Physics Manual – Describing the underlying physical models and nuclear data processing.
- Developers Manual – Description of the software architecture and integration of the Dash/OpenMC [1] [2] framework.

This document is the Physics Manual for the VERITAS simulator.

2. Theory of Neutron Moderation

Neutron moderation is the process by which high-energy "fast" neutrons (typically produced by (α, n) sources at ≈ 2 MeV) are reduced to thermal energies (≈ 0.025 eV) through successive collisions with moderator nuclei. In this simulation, we focus primarily on **elastic scattering**, which is the dominant mechanism for energy loss in light-moderator systems.

2.1. Elastic Scattering Kinematics

In an elastic collision between a neutron of mass $m = 1$ and a nucleus of mass A, kinetic energy and momentum are conserved. The ratio of the neutron's final energy (E') to its initial energy (E) is determined by the scattering cosine in the Center-of-Mass (CM) frame (μ_{cm}):

$$\frac{E'}{E} = \frac{A^2 + 1 + 2A\mu_{cm}}{(A+1)^2} \tag{1}$$

By expanding the denominator and isolating the angular-dependent term, we can express the energy ratio in a linear form:

$$E' = E\left[\frac{A^2+1}{(A+1)^2} + \frac{2A}{(A+1)^2}\mu_{cm}\right] \tag{2}$$

Under the assumption of isotropic scattering in the CM frame (s-wave scattering), all values of μ_{cm} between -1 and 1 are equally probable.

2.1.1. The Collision Parameter α

The maximum energy loss occurs during a head-on collision ($\mu_{cm} = -1$), which defines the minimum energy a neutron can retain, $E_{min} = \alpha E$. The collision parameter α is defined as:

$$\alpha = \left(\frac{A-1}{A+1}\right)^2 \tag{3}$$

Substituting α back into the kinematic equation provides the standard form used for stochastic sampling:

$$E' = \frac{E}{2}\left[(1+\alpha) + (1-\alpha)\mu_{cm}\right] \tag{4}$$

2.2. Angular Transformations and Laboratory Anisotropy

While scattering is isotropic in the center-of-mass (CM) frame, the motion of the CM relative to the laboratory (LAB) frame introduces a distinct forward-scattering bias. The LAB scattering cosine $\mu_{\text{lab}} = \cos\theta$ is linked to the CM scattering cosine μ_{cm} via the kinematic relationship:

$$\mu_{\text{lab}} = \frac{1 + A\mu_{\text{cm}}}{\sqrt{1 + A^2 + 2A\mu_{\text{cm}}}} \tag{5}$$

This transformation dictates that the neutron is physically "dragged" in the direction of its initial laboratory momentum.

To visualize this phenomenon, the **VERITAS**e supports a *Scattering Cosine/Angle PDF* routine that renders either the raw angular distribution $p(\theta)$ or its directional cosine profile $p(\cos\theta)$. Mathematically, the expected value of the directional cosine is defined as:

$$\langle \cos\theta \rangle = \int_{-1}^{1} \cos\theta \, p(\cos\theta) \, d(\cos\theta) \tag{6}$$

For single-nuclide elastic scattering, assuming exact CM isotropy, this integration reduces cleanly to

$$\langle \cos\theta \rangle = \frac{2}{3A}. \tag{7}$$

For composite molecular moderators consisting of more than one atom (such as H_2O), the software evaluates the total theoretical expectation value via a weighted linear combination across the constituent species:

$$\langle \cos\theta \rangle = \frac{1}{N}\sum_{i=1}^{N} \langle \cos\theta \rangle_i \tag{8}$$

where N is the total number of atoms in the molecular matrix [**?**].

It must be noted that while $\langle \cos\theta \rangle$ yields a exact algebraic expression, the average scattering angle itself ($\langle \theta \rangle$) has no simple, closed-form analytical solution due to the non-linear tracking transformations. The software explicitly handles the theoretical angle baseline as an approximation, highlighting the fundamental stochastic inequality:

$$\langle \theta \rangle \neq \arccos\langle \cos\theta \rangle \tag{9}$$

For light nuclei like Hydrogen ($A = 1$), $\langle \cos\theta \rangle = 2/3$, causing strong forward laboratory anisotropy that directly couples maximum momentum transfer to large deflection angles. For heavy structural absorbers ($A \gg 1$), $\langle \cos\theta \rangle \approx 0$, collapsing the system into symmetric, isotropic behavior in both frames.

2.3. Logarithmic Energy Decrement (ξ)

Because neutron energy spans several orders of magnitude, energy loss is best characterized by the change in the logarithm of energy, or lethargy. While the average energy after n collisions follows a geometric progression:

$$
\begin{aligned}
E' &= E \cdot \frac{1}{2}\left[(1+\alpha) + (1-\alpha)\mu_{cm}\right] \\
E'' &= E' \cdot \frac{1}{2}\left[(1+\alpha) + (1-\alpha)\mu'_{cm}\right] \\
&= E \cdot \left(\frac{1}{2}\right)^2 \left[(1+\alpha) + (1-\alpha)\mu_{cm}\right]\left[(1+\alpha) + (1-\alpha)\mu'_{cm}\right] \\
E^{(n)} &= E \cdot \left(\frac{1}{2}\right)^n \prod_{i=1}^{n}\left[(1+\alpha) + (1-\alpha)\mu_i\right]
\end{aligned}
\tag{10}
$$

By taking the expectation value of the n-th collision energy, and noting that for isotropic scattering in the CM frame the average scattering cosine is zero ($\langle \mu_i \rangle = 0$), the product simplifies significantly:

$$
\langle E^{(n)} \rangle = E \cdot \left(\frac{1}{2}\right)^n \prod_{i=1}^{n} \langle (1+\alpha) + (1-\alpha)\mu_i \rangle = E\left[\frac{1+\alpha}{2}\right]^n \tag{11}
$$

To relate this to the logarithmic energy decrement, let us define a stochastic variable $\xi^{(i)}$ for each collision such that:

$$
e^{-\xi^{(i)}} = \frac{E^{(i)}}{E^{(i-1)}} = \frac{1}{2}\left[(1+\alpha) + (1-\alpha)\mu_i\right]
$$

Taking the natural logarithm of the ratio between the final energy $E^{(n)}$ and the initial energy E yields an additive relationship in lethargy:

$$
\ln\left(\frac{E^{(n)}}{E}\right) = \ln\left(\prod_{i=1}^{n} e^{-\xi^{(i)}}\right) = -\sum_{i=1}^{n} \xi^{(i)} = -(\xi' + \xi'' + \cdots + \xi^{(n)}) \tag{12}
$$

Applying the expectation operator to this sum, we find the average total lethargy gain:

$$
\left\langle \ln \frac{E^{(n)}}{E} \right\rangle = -n\langle \xi^{(i)} \rangle = -n\xi \tag{13}
$$

where ξ is the mean logarithmic energy loss per collision. A more physically consistent measure of this parameter is derived by integrating over the probability distribution of the final energy E':

$$
\xi = \left\langle \ln \frac{E}{E'} \right\rangle = \frac{\int_{\alpha E}^{E} \ln\left(\frac{E}{E'}\right) \frac{1}{(1-\alpha)E} dE'}{\int_{\alpha E}^{E} \frac{1}{(1-\alpha)E} dE'} \tag{14}
$$

For a specific isotope, ξ is independent of the incident energy and depends only on A:

$$
\xi = 1 + \frac{\alpha \ln \alpha}{1-\alpha} \tag{15}
$$

For heavier nuclei ($A > 10$), this is commonly approximated by the Taylor expansion:

$$
\xi \approx \frac{2}{A + 2/3} \tag{16}
$$

In the simulation, deviations from this constant at low energies indicate the onset of **thermal upscattering**, where the target nucleus's kinetic energy can no longer be overlooked, leading to a net decrease in ξ as the system approaches equilibrium.

By inverting this expectation value, the relationship can be rearranged to directly calculate the theoretical average number of collisions $\langle n \rangle$ required for a fast neutron with an initial energy E_0 to decelerate down to a given thermal threshold E_{th}:

$$\langle n \rangle = \frac{\ln\left(\frac{E_0}{E_{\text{th}}}\right)}{\xi} \tag{17}$$

For a typical fission neutron born at $E_0 = 2$ MeV thermalizing to $E_{\text{th}} = 0.0253$ eV in hydrogen, the total required lethargy change is fixed at $\ln(E_0/E_{\text{th}}) \approx 18.2$. Consequently, the average collision count scales inversely with ξ, which is the property of the moderating material. Light water ($\xi \approx 0.707$) requires an average of roughly 26 collisions, whereas a heavier moderator like graphite ($\xi \approx 0.158$) shifts this threshold significantly upward to approximately 115 collisions.

2.4. Thermal Neutron Upsscattering: Real vs. Idealized Media

Neutron upscattering occurs in the low-energy thermal regime ($E \leq 1$ eV), where a neutron gains kinetic energy during a scattering collision. This behavior marks a major divergence between real physical moderators and the idealized material models generated within the VERITAS framework.

2.4.1. Upsscattering in Real Moderators

In a real-world moderator at a finite temperature T (such as light water at 300 K), the target nuclei are not stationary. They possess random thermal kinetic energy governed by a Maxwell-Boltzmann velocity distribution. When a slow thermal neutron collides with a moving target nucleus, energy can be transferred from the vibrating nucleus back to the neutron, increasing the neutron's velocity ($E' > E$).

In state-of-the-art simulations, this is governed by the principle of **detailed balance**, which balances upscattering and downscattering probabilities in thermodynamic equilibrium:

$$\Sigma_s(E \to E')M(E) = \Sigma_s(E' \to E)M(E') \tag{18}$$

where $M(E)$ represents the Maxwellian flux spectrum. To model this accurately, OpenMC relies on explicit, pre-calculated thermal scattering libraries ($S(\alpha, \beta)$) that account for molecular binding forces and ambient lattice vibrations.

2.4.2. The Absence of Upsscattering in Idealized Moderators

In contrast, the idealized materials programmatically generated by the `pydecs.py` [3] module do not exhibit upscattering.

These virtual nuclides are modeled using raw potential scattering cross-sections that treat target nuclei as perfectly stationary, cold targets (effectively at 0 K). Because the generation pipeline deliberately bypasses NJOY's [4] Doppler-broadening (`BROADR`) step to keep the idealized mathematical shapes (like step-function windows) perfectly crisp, no thermal velocity is assigned to the target matrix. Because a stationary nucleus has no kinetic energy to yield, a colliding neutron can never gain energy. As a result, neutrons in these idealized media experience only energy loss via downscattering or energy conservation via static elastic scattering.

2.5. The $1/E$ Slowing Down Spectrum

In an infinite, non-absorbing medium with a constant source of fast neutrons, the balance of neutrons slowing down leads to a characteristic flux distribution $\Phi(E)$. The probability of finding a neutron in a specific energy interval is inversely proportional to that energy:

$$\Phi(E) = \frac{S}{\Sigma_s \xi E} \tag{19}$$

where S is the source strength and Σ_s is the macroscopic scattering cross-section. This analytical $1/E$ relationship provides the theoretical baseline for the dN/dE spectral plots. Discrepancies between the simulation and this model typically arise from energy-dependent cross-section resonances or the transition into the thermal Maxwellian distribution.

2.6. Maximum and Average Energy Loss per Collision

The simulator tracks neutron energy attenuation via a $\Delta E/E$ vs. initial energy pipeline. The relative energy loss per collision is defined as $\frac{\Delta E}{E} = \frac{E_{\text{in}} - E_{\text{out}}}{E_{\text{in}}}$. For elastic scattering off a target nucleus of mass number A, the maximum possible relative energy transfer occurs during a head-on collision:

$$\left(\frac{\Delta E}{E}\right)_{\max} = 1 - \alpha, \quad \text{where} \quad \alpha = \left(\frac{A-1}{A+1}\right)^2 \tag{20}$$

Assuming isotropic scattering in the center-of-mass frame, the average relative energy loss is exactly half of this maximum limit: $\left\langle \frac{\Delta E}{E} \right\rangle = \frac{1-\alpha}{2}$.

2.7. Energy Transfer Probability and the Scattering Kernel

While the previous sections define the average energy loss per collision, the Monte Carlo simulation requires a specific probability density function (PDF) to sample the exact energy E' after a collision.

For elastic, isotropic scattering in the CM frame, the probability of a neutron with initial energy E scattering into a unit energy interval around E' is known as the scattering kernel, $P(E \to E')$. Since the scattering cosine μ_{cm} is distributed uniformly between -1 and 1, the resulting energy distribution is also uniform within the kinematically allowed range $[\alpha E, E]$:

$$P(E \to E') = \begin{cases} \frac{1}{(1-\alpha)E} & \text{for } \alpha E \le E' \le E \\ 0 & \text{otherwise} \end{cases} \tag{21}$$

This "box" distribution implies that for a single collision, any final energy state within the allowed limits is equally probable.

2.7.1. Asymptotic Slowing Down Density

The $1/E$ relationship observed in the simulation's spectral plots is a direct mathematical consequence of this uniform scattering kernel. In a non-absorbing medium, the number of neutrons slowing down past a certain energy per unit time must be constant. If we define the collision density $F(E')$ as the number of scattering interactions per unit energy, the integral equation for the slowing-down density is:

$$F(E') = \int_{E'}^{E'/\alpha} F(E) P(E \to E') dE = \int_{E'}^{E'/\alpha} \frac{F(E)}{(1-\alpha)E} dE \tag{22}$$

The solution to this integral equation in the region well below the source energy is the asymptotic distribution:

$$F(E') = \frac{S}{\xi E'} \tag{23}$$

This confirms that the $1/E$ flux distribution ($\Phi \propto 1/E$) arises because the probability of a neutron "landing" in a specific energy interval dE' is inversely proportional to the width of the scattering interval $(1-\alpha)E$ from which it originated.

2.7.2. Isotopic Influence on the Kernel

The width of this probability ”box” is governed by the mass of the moderator A:

- **Hydrogen ($A = 1$):** Since $\alpha = 0$, the kernel $P(E \to E') = 1/E$ covers the entire range from 0 to E. The probability is perfectly flat, meaning a single collision can thermalize a fast neutron.
- **Heavy Nuclei ($A \gg 1$):** The interval $(1-\alpha)E$ becomes extremely narrow. The probability density $1/((1-\alpha)E)$ becomes very large over a tiny energy range, meaning the neutron's energy E' after collision is almost guaranteed to be very close to its initial energy E.

3. Neutron Population Dynamics

Monitoring the total number of active neutrons, $N(t)$, provides a macroscopic view of the simulation's progress. While individual histories are stochastic, the population as a whole follows predictable decay patterns governed by the medium's properties and the system's geometry.

3.1. The Mean Lifetime τ

The simulation provides a functional fit for the population decay using the standard survival equation:

$$N(t) = N_0 e^{-t/\tau} \tag{24}$$

In this context, τ is the **mean lifetime** of a neutron. It represents the average time a neutron exists in the simulation before being removed. This removal occurs through two independent mechanisms:

3.1.1. Removal Mechanisms

- **Absorption:** The neutron is captured by a nucleus, a process governed by the macroscopic absorption cross-section Σ_a. The probability of absorption per unit time is given by $\lambda_{abs} = \Sigma_a v$.
- **Leakage:** The neutron crosses the geometric boundaries of the simulation and is no longer tracked. In diffusion theory, this is modeled by the geometric buckling B^2 and the diffusion coefficient D, where the probability of leakage per unit time is $\lambda_{leak} = DB^2 v$.

The total decay constant extracted by the simulation fit is the inverse sum of these probabilities:

$$\frac{1}{\tau_{total}} = \frac{1}{\tau_{abs}} + \frac{1}{\tau_{leak}} = v(\Sigma_a + DB^2) \tag{25}$$

3.2. Velocity Approximation

This equation assumes that the neutron velocity v is constant, which is physically non-trivial since neutrons undergo significant energy loss during moderation. However, in this simulation framework, the exponential model remains a valid approximation. Because the time required for a neutron to moderate from high energies (e.g., 2 MeV) to the thermal floor is negligible compared to the time it spends diffusing at thermal equilibrium, the velocity effectively stabilizes. Consequently, the bulk of the $N(t)$ curve reflects the decay of a population at a nearly constant, thermalized velocity.

4. Mean Free Path (λ)

The mean free path is the average distance a neutron travels between successive interactions (collisions). In the Monte Carlo framework, this parameter is critical for determining the step size of a neutron's trajectory within the medium.

4.1. Mathematical Definition

The mean free path is inversely proportional to the total macroscopic cross-section Σ_t of the material. It is calculated as:

$$\lambda = \frac{1}{\Sigma_t} = \frac{1}{N\sigma_t} \tag{26}$$

Where:

- N is the atomic number density of the moderator (atoms/m^3).
- σ_t is the microscopic total cross-section (m^2).

4.2. Application in Simulation

In the simulation, the mean free path is used to determine the distance s to the next collision site. Since neutron interactions are stochastic, the distance s is sampled from an exponential probability distribution:

$$p(s)ds = e^{-\Sigma_t s}\Sigma_t ds \tag{27}$$

Using a random number $\xi \in [0, 1)$, the step length is computed as:

$$s = -\lambda \ln(\xi) \tag{28}$$

4.2.1. Physical Significance and Transport Regimes

The magnitude of λ relative to the system's characteristic dimension (e.g., the radius R) determines the transport regime of the neutrons. In high-density moderators at cryogenic temperatures, the microscopic cross-section σ_t is high, resulting in a mean free path that is typically orders of magnitude smaller than the system boundary ($\lambda \ll R$).

This disparity creates a **diffusive regime**: instead of "streaming" directly toward the boundary, neutrons undergo a dense random walk. Each collision resets the neutron's direction, effectively "trapping" it within the medium. This drastically increases the neutron's residence time and total path length, explaining why the population can persist for seconds even within a physically small volume.

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