Design of an Optical Medium for the Simulation of Neutron Transport in Reactor Component Materials

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Abstract

The scattering of optical rays by small spherical particles bears a strong resemblance to the diffusion of fission neutrons in solid materials. This work explores the feasibility of exploiting similarities between these two systems for the purposes of reactor component analysis, education, and outreach. After a brief overview of reactor-environment neutronics, an easily-producible optical scattering medium is proposed and examined for its ability to faithfully simulate scattered neutron distributions and energy deposition patterns in three dimensions. Individual scattering particles (3M Spherical Glass Microshells) are probed for their ray-scattering properties, and a random-walk simulation reveals how an iterated scattering process could be used to imitate scattering angle probability distributions for given materials. In the optical system, iterated angular probability distributions are shown to evolve in similar fashion to neutron scattering angle distributions with respect to atomic mass number, and further quantitative relationships are established between the disparate systems. Stopping short of a final optical test for correlation with accepted benchmark simulations, thorough groundwork is laid for future experiments. Methods and materials are discussed in detail, and possible end-use applications are considered.

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1. Background

1.1. An Optical Simulation Tool for Reactor Component Modelling

Neutron scattering and diffusion are fundamental elements of nuclear reactor theory which allow engineers to predict rates of reaction and other operation parameters. Despite the many complexities inherent to neutron-nucleus interactions and their macro-scale statistical analyses, problems in neutron diffusion are commonly reduced in a series of approximations to partial differential distributions such as the three-dimensional Helmholtz equation so often applied to wave theory.

The impetus for this text and the following experiments arose from observations of the mathematical similarities shared by electromagnetic scattering and neutron diffusion. The notion of exploiting this similarity for application to nuclear research seems appropriate to consider, despite that a number of computational tools already exist for diffusion and reactor analysis. This manuscript will cover the design, testing, and possible use of an easily-manufacturable optical scattering medium for the simulation of neutron distribution and fission energy transport in simulated reactor components.

Benchmark nuclear engineering software such as the commonly-used Monte Carlo N-Particle Transport Code (MCNP) has made accessible the simulation of nuclear processes to those with advanced training. At the same time, the principles of reactor dynamics and nuclear science in general remain esoteric to all others with less formal education. Without an understanding of differential mathematics or particle interaction, the majority are left without access to the main concepts of nuclear physics and reactor operation. The result of this is a low level of public awareness and widespread misconception with regard to the transport, use, and handling of fissile materials.

A hands-on interactive learning tool that demonstrates the basic tenets of reactor design and control through visual means could be a valuable educational aid which could be geared toward audiences varying in levels of education. Like reactor control simulator software available today, a visual model would give learners a uniquely engaging experience with reactor kinetics and the basic ideas behind nuclear energy. For example, one might imagine a set of mock reactor components which are illuminated by color according to neutron population density and fission energy release. The set might be connected to reactor simulator software of any degree of complexity, while the individual components could be manipulated by hand on an inductive-charging surface. A kit such as rendered in Figure 1 may find purpose in educational outreach, the classroom, or the engineering boardroom.

In addition to having applications in education and outreach, it is possible that an optical scattering model with sufficient accuracy could be of some use in thermal or reactivity analysis as it applies to component design. Though it is currently possible to import solid models into MCNP and other such programs for analysis, it may not often be practical to include intricate geometries such as found in fasteners, threads, springs, or other such components. If an optical model were capable of faithfully mapping neutron diffusion or heating by neutron or gamma energy deposition, any object cast or machined from the scattering media might be probed or photographed for optical intensity to identify any potential hot-spots or reactivity concerns.

Figure 1. A hypothetical interactive set of model reactor components that interface with reactor simulator software, giving real-time optical feedback
1.2. Overview: Concepts in Neutron Transport Modelling

Spatial neutron distribution and spatial energy deposition are the primary reactor processes that lend themselves to optical simulation. The scope of this text will be restrained by sidestepping some of the more detailed aspects of both optical and neutron scattering, though all necessary mentions will be made of the underlying laws and conventions which will apply. The entire model will benefit from a series of convenient approximations which arise from the systems at hand. Readers familiar with reactor physics may already anticipate that certain aspects of neutron interaction will not lend themselves to reproduction in a steady-state optical medium (e.g., time-evolved temperature and energy dependence of interaction cross sections). These concerns will be addressed as constraints emerge through physical considerations and intended goals for a final model.

As a qualitative preliminary estimate, conformity of the optical models to accepted benchmarks using the methods and materials as laid out in this manuscript could be expected to lie in the 70-90% range. Though a final benchmark correlation will not be found in the scope of this work, some quantitative conclusions will be drawn as to the efficacy of the methods proposed, as well as suggestions on how they may be improved before final testing.

1.2.1. Neutron Scattering and Cross-Sections

Before considering how specifically to model spatial neutron distribution and energy deposition, we first examine the relatively straightforward matter of neutron interaction statistics. The neutron is both a product of nuclear fission and the catalyst for new fission events. The business of controlling the nuclear chain reaction is, in its simplest form, a matter of controlling the spatial distribution of fission neutrons so that on average at least one neutron from each fission event remains “in play” long enough to trigger another event. Much of the bulk material comprising the reactor is designed to moderate the speed of fission neutrons or to allow them to escape in a controlled fashion. The instantaneous distribution of neutrons within the reactor core is directly related to the rate at which the chain reaction is sustained, and must be optimized for proper control authority, heat generation, and fuel consumption.

As the neutron itself is charge-neutral, it interacts with electrostatic potentials only weakly through its very slight intrinsic magnetic moment. Thus, the neutron is capable of penetrating matter with a mean free path on the order of centimeters. What few interactions do occur are almost exclusively with atomic nuclei. Whether or not an interaction occurs, and to what degree, is largely a function of the neutron’s incident energy and the internal energy structure of the nucleus. The nuclide (the nucleus of any particular atomic species), is characterized by distinct energy eigenvalues corresponding to possible nucleon configurations and so must be treated energetically with the application of quantum mechanics and perturbation theory. This is true except in the case of the heaviest elements, whose higher state densities lead energy quanta to behave more classically. In essence, the possible energy states of the nucleus determines its tendency to interact with a neutron at a particular energy. That tendency, or probability of interaction, is plotted in a manner such as the one for elastic neutron scattering by \(^9\)Be in Figure 2. Engineers take a practical approach to the statistics that follow by treating these probabilities as “resonance cross sections”, and assigning the nucleus a pseudo-physical cross-sectional area having units of barns \((1b = 10^{-24} cm^2)\). Together with the material’s density, the cross section serves to describe the average likelihood of a collision within a given distance travelled by the neutron. If \(I(x)\) describes an average beam intensity of uncollided neutrons after travelling \(x\) cm into a solid material,

\[
I(x) = I_0 e^{-N\sigma x} = I_0 e^{-\Sigma x},
\]

where \(N\) represents the density of neutrons per \(cm^3\), and \(\sigma\) is the generalized microscopic collision cross section in barns. Multiplied together, these variables give the total macroscopic collision cross section \(\Sigma\) which has units of \(cm^{-1}\), and an inverse \(1/\Sigma\) which equals the average mean free path, often labelled \(\lambda\).
When interactions occur, several outcomes may follow. Scattering may be elastic or inelastic, or have properties of both which may be influenced by thermal energy of the substrate. Absorption by the nucleus can also occur, which may be permanent or temporary. Absorption can also lead to a fission event in radionuclide interactions. Any species the experimenter may wish to bombard with neutrons is characterized by its associated microscopic and macroscopic resonance cross section curves, and each of the collision outcomes is given its own effective cross section which varies individually by incident neutron energy (Table 1). Each cross section is influenced to a certain degree by substrate thermal motion. The effect of temperature is usually small compared to that of incident neutron energy, but it does provide the reactor with negative feedback by shortening and broadening peaks present in the resonance curve. This “Doppler broadening” is described by simple application of a Maxwell-Boltzmann distribution, and gives relative neutron-nucleus energies. Further mention of the subject follows in section 1.2.4.

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### Table 1: Various Microscopic Neutron Interaction Cross Sections

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Constituents</th>
<th>Relationship</th>
</tr>
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<tbody>
<tr>
<td>σₐ</td>
<td>Scattering cross section</td>
<td>σₐ  Elastic scattering cross section</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>σₐ'  Inelastic scattering cross section</td>
<td></td>
</tr>
<tr>
<td>σₐ</td>
<td>Absorption cross section</td>
<td>σ₇  Capture cross section</td>
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<td></td>
<td></td>
<td>σ₇'  Fission cross section</td>
<td></td>
</tr>
<tr>
<td>σₜ</td>
<td>Total cross section</td>
<td>σₜ  Scattering cross section</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>σₐ  Absorption cross section</td>
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1.2.2. Neutron thermalization

Much of the effort of designing a reactor goes into predicting and controlling spatial neutron distributions. Part of the problem is preventing the escape of fast fission neutrons before they have chance to precipitate further reactions. By strategic placement of moderating materials, fast neutrons are slowed and spatially restricted in a series of collisions, each diminishing their kinetic energies by an average of $\xi E$, where $\xi$ is known as the slowing-down decrement $^3$.

$$\xi = \ln(E / E') \approx \frac{2}{A + 2/3}.$$  \[2\]

where $A$ is the atomic mass number of the target nucleus. As per this approximation, we see that the lighter elements provide the greatest moderating effect. Neutron kinetic energies are often broken down by regime, where fast $>$ epithermal $>$ thermal. In the reactor environment, these energies may range widely from $\sim 2$MeV in the fast regime to $\sim 0.025$eV in the thermal. Using $\xi$, the number of elastic collisions $n$ necessary to slow a neutron from $E_0$ to $E_n$ can be averaged $^3$.

$$n = \frac{1}{\xi} \ln (E_0 / E_n)$$  \[3\]
For example, solving for \( n \) in hydrogen and moving from 2MeV to 0.025eV gives \( n \approx 15 \). Because heavier nuclei absorb less kinetic energy per collision, this number increases with \( A \). As cross sections vary accordingly to energy, mean free paths are also adjusted. Because interaction cross sections and mean free paths vary widely across energy groups, many calculations in engineering benefit by treating them separately, ignoring groups when necessary. For example, thermal neutrons occupying one region of space will not affect regions farther than one mean free path \( \lambda = 1 / \Sigma \), which is much shorter than the mean free path of a fast fission neutron. More on energy group approximation follow in sections 1.2.4 and 1.3.3.

1.2.3. Neutron scattering angles
It is essential to understand the kinematics and statistics of elastic neutron scattering in both the center of mass (CM) and laboratory (LAB) reference frames. Figure 3 illustrates the labelling of initial and resultant velocities and angles in both systems. All of the following figures assume a nucleus starting at rest.

\[
\frac{E'}{E} = \frac{\frac{1}{2}mv'^2}{\frac{1}{2}mv^2} \quad \Rightarrow \quad E' = \left[ \frac{(1+\alpha) + (1-\alpha) \cos \theta_{CM}}{2} \right] E
\]

Equations 4 and 5 arise from the geometry of the system and give us a resultant neutron kinetic energy \( E' \) in terms of initial energy \( E \) and the CM scattering angle \( \phi_{CM} \), where \( \alpha \equiv (A - 1 / A + 1)^2 \). This is informative and useful for energy calculations, but measurements of the geometry of neutron scattering and diffusion are made in the laboratory frame. Geometry provides us with relations (Fig. 4) between CM and LAB scattering angles (Eq. [6], [7], [8]).

\[\text{Figure 3. Elastic scattering angles as defined in the center of mass and lab reference frames (Source: Duderstadt)}\]
\[ v'_{LAB} \sin \theta_{LAB} = v'_{CM} \sin \theta_{CM} \]  
\[ v'_{LAB} \cos \theta_{LAB} = v'_{CM} \cos \theta_{CM} + v_{CM} \]  
\[ \tan \theta_{LAB} = \frac{v'_{CM} \sin \theta_{CM}}{v_{CM} + v'_{CM} \cos \theta_{CM}} \]  
\[ = \frac{\sin \theta_{CM}}{\Lambda + \cos \theta_{CM}} \]  

For use in the many integro-differential representations of neutron flux, current, and density, it is often useful to characterize observables as functions of one another. The cross section \( \sigma \) in either frame can be expressed as a function of scattering angle \( \theta \) since the two are energetically linked. The scattering cross section in the CM frame as a function of resultant angle is then \( \sigma_s(\theta_{CM}) = d\sigma_s / d\Omega_{CM} \), where \( \Omega_{CM} \) is the unit vector in the direction of resultant neutron motion. The physical meaning of the differential \( d\sigma_{CM} / d\Omega_{CM} \) can be understood as the probability of a scattering event ranging by resultant neutron direction vector. This generalization is true in both reference frames and can also be related by energy to the cross sections \( \sigma_s(E) \) (Fig. 2).

In the CM “s-wave” scattering regime, we have an isotropy with respect to resultant angle. This leads to

\[ \frac{d\sigma_s}{d\Omega_{CM}} = \sigma_s(\theta_{CM}) = \sigma_s(E) \frac{1}{4\pi}. \]  

Since probabilities of interaction are frame-invariant, and since the differentials \( d\sigma_{CM} / d\Omega_{CM} \) and \( d\sigma_s / d\Omega_{LAB} \) vary equivalently, angular distributions in cross section can be moved from frame to frame by differential manipulation;

\[ \sigma_s(\theta_{LAB}) d\Omega_{LAB} = \sigma_s(\theta_{CM}) d\Omega_{CM} \]  
\[ \Rightarrow \sigma_s(\theta_{LAB}) = \sigma_s(\theta_{CM}) \frac{\sin \theta_{CM}}{\sin \theta_{LAB}} \frac{d\theta_{CM}}{d\theta_{LAB}}. \]  

Thus we have related the CM and LAB differential scattering cross sections by

\[ \sigma_{LAB}(\theta_{LAB}) = \sigma_{CM}(\theta_{CM}) \frac{1 + \frac{2}{\Lambda} \cos \theta_{CM} + 1}{1 + \frac{2}{\Lambda} \cos \theta_{CM}}^{3/2}. \]  

Using Equation 9 and knowing the relationship between \( \theta_{CM} \) and \( \theta_{LAB} \), we arrive at an equation that relates the scattering cross section and resultant scattering angle in the LAB frame:

\[ \mathbb{P}(\theta_{LAB}) = \sigma_s(E) \frac{1 + \frac{2}{\Lambda} \cos \theta_{CM} + 1}{1 + \frac{2}{\Lambda} \cos \theta_{CM}}^{3/2}, \]  

where \( \theta_{CM} \) is expressed as a first-quadrant solution to Equation 8;
The LHS of Equation [13] likens the differential scattering cross section to the probability of interaction by \( \sigma_{LAB}(\theta_{LAB}) = \delta_{LAB} \delta(\theta_{LAB}) \), where the unit vector in \( \sigma \) space \( \delta_{LAB} \) is dropped. Equation 13 gives a plot of probability vs scattering angle. The distribution is strongly forward-biased when the target nuclide is very light. By application of the “single-speed diffusion approximation”, which will be discussed in the next section, angular distribution approaches isotropy with increasing \( A \) by the average-value relation \( \langle \cos \theta_{LAB} \rangle = 2/3A \).

### 1.2.4. Assumptions and Approximations

The optical model will rely on several approximations relating to both optical scattering and neutron diffusion theory. In particular, since the model as currently conceived would not have the ability to alter its scattering cross sections based on any analog for incident neutron energy, a single cross section will need to be assumed based on an average speed. As it happens, computational analysis on neutron population in solid volumes is commonly simplified by that very assumption. This is referred to as the single-speed diffusion model, and preliminary design estimates have long been gained through its application, wherein energy dependence is eliminated by assuming a single neutron energy and treating transport as a simple diffusion process.

Since the goal of this work is to gauge correlation with more accurate numerical methods, it will not necessarily serve to derive the differential mathematics of the single-speed diffusion approximation or to directly solve the associated partial differential equation. Instead, we will examine attributes of the approximation and attempt to emulate them in the optical system.

The end result of the single-speed approximation is the Helmholtz equation

\[
-D \nabla^2 \phi(r) + \Sigma_a \phi(r) = S(r),
\]

where \( D \) is a diffusion coefficient related to the mean free path, \( \Sigma_a \) is the macroscopic absorption cross section, \( \phi(r) \) is a scalar neutron flux term given as a function of position only, and \( S(r) \) is a neutron source term and is also a function of position. Further definition of these variables can be found in popular introductory nuclear engineering texts, but here a brief mention of the equation will suffice in order to frame the arguments on which it leans. Those arguments, along with their implications for the optical model, follow here:

1. **Time-invariance** The Helmholtz equation has only steady-state solutions. This approximation implies that the volume in question has no properties which can change in time. Temperature-dependent properties of the substrate are thereby restricted to a single value. The optical model plays into this scheme by design, since a passive optical medium and a constant source would be employed. If time-dependent properties such as reactivity feedback are desired for future simulation applications, they would need to be achieved through programmatic modulation of source intensity.

2. **Homogeneity** The equation assumes that the diffusion coefficient \( D \) and the macroscopic absorption cross section \( \Sigma_a \) are constant with respect to position. While the experiments carried out in this work will fit this condition by using only uniform optical media, the criteria is not in any way a restriction on other experiments which may be performed. It is only to say that the Helmholtz equation will provide physically meaningful solutions when the region in question is uniform. In theory, separate optical media which individually comply with the Helmholtz distribution could be joined in any arrangement and the physics of the system would play out in agreement with another more advanced mathematical description.
3. Single neutron energy The Helmholtz equation is the homogeneous, time-invariant version of the single-speed neutron transport equation. As previously mentioned, the optical medium would be restricted to a single macroscopic scattering cross section analog. Therefore, a single neutron energy would need to be chosen for each physical model, and a single energy group’s final population distribution would be found. Since the Watt neutron flux spectrum (Fig. 5) gives an average kinetic energy of around 2MeV for fission neutrons, a cross section analog could be created which corresponds to that particular energy as per a published resonance cross section curve like the one in Figure 2. By default, the single-speed approximation does not account for energy augmentation caused by thermal motion of nuclei, but application of Maxwell-Boltzmann statistics can accomplish this. If desired, statistics can be applied to adjust the cross sections for Doppler broadening at a given temperature as described in section 1.2.1. For the purposes of this work, however, impacts of thermal motion will be considered negligible.

The Watt Fission Neutron Flux Spectrum

![Figure 5: The Watt fission neutron flux spectrum, indicating an average neutron energy of approximately 2MeV (Source: CERN)](Image)

4. Linear anisotropy Note that $\phi(r)$ is a scalar neutron flux, as opposed to an angular neutron flux. Hence, it carries no information on neutron direction. This reflects a mathematical simplification made in the derivation of the single-speed diffusion approximation wherein it was assumed that the angular neutron flux, denoted in the original neutron transport equation as $\phi(\vec{r}, E, \hat{\Omega}, t)$, was only *weakly* dependent on angle. That is to say, the angular flux $\phi$ changes very little (and only linearly) with respect to the direction vector $\hat{\Omega}$. This assumption can be considered true for the purposes of Equation 15 in most cases within the bulk of a material where diffusion and backscattering are in progress. The assumption does not hold true near boundaries where directionality is more pronounced, near sources, or in strongly absorbing media where flux varies greatly in spatial increments on the order of a mean free path. Linear anisotropy is an approximation made in formulating the equations of the one-speed model and does not represent a physical constraint with regard to experiment. Implications of this assumption on the optical model do restrict the use of any highly-absorbing substrate. Accordingly, initial tests should utilize optical media with a very low extinction coefficient. This would effectively nullify the second term in the Helmholtz equation, but it should also be possible to increase the extinction coefficient with absorptive agents to simulate the absorption cross section of a given material.
5. **Isotropic source term** Fission neutron sources are for all intents and purposes considered perfectly isotropic. Any simulation of neutron distribution will also need an isotropic source. This can be accomplished in the optical model by the use of a highly diffusive lens or layer of dense scattering media at the source aperture. The source aperture should also be defined as isotropic in the MCNP simulation which will be used to check for conformity of the model. Further description of experimental methods will be found in section 2.2.

1.3. **Features of a Functioning Optical Model**

1.3.1. **General Optical Properties**

After examination of the one-speed diffusion model, which according to the literature\(^1\) yields results accurate at least to first order, we have identified several properties of an appropriate optical model.

A. The test model should operate and be measured in the steady state. This is easily accomplished by measuring time-averaged light intensities and using a constant source.

B. Until a satisfactory composition of optical media is found, the model should use homogeneous distributions of scattering agent within the suspending substrate. Further experimentation with inhomogeneous media and/or discontinuous boundaries may be attempted in future work.

C. The model must use optical media having a low coefficient of extinction. This should be simple to assume if a very transparent resin substrate and relatively non-absorbing glass particles are used, especially at length scales in centimeters. If the test article is to attempt to replicate a material having a low but non-zero absorption cross section, an appropriate concentration of absorptive particulate may be added. Section 2.2 will outline this technique.

D. The model must employ an isotropic source. This should be easily approximated through the use of either a highly diffusive lens or the integration of a highly scattering layer at the boundary of the source aperture. In addition, computer modelling should also assume an isotropic source region.

Keeping these goals in mind, a few more considerations should be made with regard to optical systems.

E. The suspending substrate must be optically isotropic. Any birefringence will result in scattering angles being dependent on initial direction with respect to the resin.

F. To simulate vacuum boundaries, any internal reflections must be prevented. Total internal reflections must especially be avoided, as they would eventually be detected somewhere on a measuring surface. Any surfaces that are not to be measured should be treated with an absorptive layer.

G. Diffraction within the medium should be accounted for, and care should be given to assure that any interference patterns remain negligible on pertinent scales of measurement. The isotropic source stipulation should aid in the prevention of diffraction patterns produced by the source aperture, since this type of interference is most pronounced when the source wave is planar. The only remaining source of diffraction patterns would involve the scattering particles themselves. This will be further examined in sections 2.1 and again in 2.2.1.

H. Polarization of all light within the system can be assumed random, and does not impact intensity at scales pertinent to measurement. The topic will hence be ignored.

1.3.2. **Scattering Behavior Replication**

Perhaps the most important feature of a photonic system which mimics neutron scattering, which has yet been left unmentioned, is its ability to scatter light as neutrons are scattered within the bulk material. Having surveyed some of the pertinent background material, we move straight to a simple conclusion: a scattered ray of light within the optical medium must be deflected by an average angle matching that of the material being modelled. This must occur on average once per mean free path. The average scattering angle and the mean free path are determined by neutron energy and the material being modelled.
To illustrate, we have quantified in Equation 1 the number of collisions which occur per unit distance within the material, and found the mean free scattering path $\lambda_s = 1/\Sigma_s = 1/\sigma N_p$ where $N_p$ is the density of scattering nuclei per cm$^3$ and $\sigma = \sigma(E)$ is the effective scattering cross-sectional area of a single nucleus. $\sigma_s(E)$ is published for many common materials in the form of resonance curves for specific types of scattering and absorption interactions over a range of incident neutron energies. The optical model could easily replicate the macroscopic cross section and the mean free path by using the actual cross-sectional area of a single scattering particle for $\sigma_s$ and adjusting appropriately the density of optical scattering particles $N_p$ to match $\Sigma_e$ of the material at the chosen neutron energy.

Also associated with each scattering event is the deflection of the neutron (or ray, in the optical model) by a certain scattering angle $\theta_{LAB}$ which is given as a probability distribution in Equation 13 and depends on $\sigma_s(E)$ and $A$ of the material. To begin the search for an effective scattering agent, this work will analyze the scattering properties of an inexpensive scattering particle powder in the form of 3M brand K15 glass microbubbles. These are thin-walled spherical shells of glass with diameters on the order of 60 $\mu$m. As will be shown in section 2, the scattering angle probability distribution for a single scattering particle embedded in the chosen substrate is highly forward-biased and will not match the desired neutron scattering angle distribution of any known material. However, by application of a multiplication factor $X$ to the particle density $N_p$, the number of collisions per mean free path will be increased until the desired scattering angle probability distribution is reached. The factor $X$ will be found by computational analysis of a random walk, using repeated applications of an empirical scattering angle distribution found for K15 glass microshells.

To explain this reasoning more succinctly, the properties of the material to be modelled will provide the mean free path $\lambda_s(\sigma_s(E),A,N_p)$, as well as a target scattering angle distribution $\mathbb{P}(\theta_{LAB}(\sigma_s(E),A))$. Within the same mean free path inside the optical media, a ray will need to undergo an average of $X$ scattering events to obey a scattering angle distribution matching (as closely as possible) the probabilistic angular distribution of the material. In this manner, a ray will have been deflected by an average angle within a mean free path which is the same average deflection angle $<\theta_{LAB}>=\cos^{-1}(2/3A)$ given in section 1.2.3. Because the optical media will require multiple events per neutron MFP, a difference exists between the two systems which will likely affect end results to some unknown degree (Fig. 6).

**Figure 6:** In the neutron distribution model, a desired average scattering angle within a mean free path will be attained in a series of $X$ scattering events. In ordinary neutron scattering, this angle is reached in a single event. Therefore, a difference between the two systems exists that may likely affect end measurements.

Finally, regarding the steady-state pattern of optical intensity and its correlation with neutron distribution on a given measurement plane or surface, we must identify the energy group whose spatial distribution is being detected. Any final correlation between the intensity pattern and MCNP distribution model will need to occur after an identical number of average mean free paths traversed. To achieve this, the MCNP model should contain the optical test piece’s exact dimensions. Neutrons exiting at the measurement surface can then be classified by energy.
In order to assume that a measured intensity pattern represents the neutron population of a certain energy group, it must also be assumed that the mean free path \( \lambda_s(\sigma_s(E), A, N_n) \) of a neutron undergoing repeated collisions falls off slowly enough at pertinent length scales such that changes in \( \sigma_s(E) \) can be neglected. This should hold true for materials having smoothly varying resonance curves, but will cease to apply after several mean free paths. By this reasoning, the dimensions of the optical media could be restricted to a few multiples of \( \lambda_s \), thus improving somewhat on the single-speed approximation. Practically speaking, an optical distribution model made for use in the educational applications previously described should already fit this restriction as part thicknesses would be less than one mean free path. Length and width dimensions could be made 1:1 with actual reactor components or scaled down if desired. If fully-thermalized energy group distributions are to be modelled, part thicknesses could still be scaled to the full axial and radial dimensions; this would only mean that the model would rely more heavily on the single-speed approximation.

2. Experimental Method
The overall experimental method for the spatial neutron distribution model begins by examining the light-scattering properties of the chosen scattering agent. A cursory ray-tracing analysis is discussed, but an experimental approach is ultimately applied. Using empirical data as a starting point, a random-walk simulation is performed in a Mathematica script that yields deflection angle probability curves after \( n \) scattering events. Plots of theoretical angular distributions (solutions of Equation 13) are then generated and compared with the random walk distributions in an effort to determine whether the iterative optical scattering model is capable of reproducing targeted distributions. Finally, detailed suggestions are made with regard to a final experimental procedure, and recommendations are made for attaining best results.

Detailed suggestions are also made for testing the energy deposition model. Preparation for this experiment is less involved, since scattering within the medium is not simulated. Instead, only the first collision of an incident ray is marked and measured. A target material is proposed, and a plan for replicating its absorption and scattering cross sections is discussed.

2.1. Optical Ray Tracing in Spherical Glass Microshells

The scattering particle chosen for this initial analysis is a hollow spherical shell of soda-lime-borosilicate glass, manufactured by 3M (Fig. 7). The product was chosen for its low cost and ease of procurement, as well as for its relatively uniform light scattering properties when averaged over many small particles. Particle diameters\(^6\) for this particular product grade (K15) range from around 30-115\( \mu m \), with the 50th percentile centered at 60\( \mu m \). Shell thicknesses\(^7\) average 0.70\( \mu m \) (700\( nm \)). With this thickness on the order of approximately two wavelengths of the chosen source light, it is appropriate to question whether simple ray tracing should provide an adequate picture of scattering taking place. Since one aim of the experiment is to operate under the assumption that all diffraction effects are negligible, a comparison will be made between a simple ray-tracing analysis and an empirical scattering intensity vs angle curve. Figure 8 gives the basic geometry of the problem at hand.
A numerical account of reflections and transmissions of an actual-thickness glass shell in air was made via spreadsheet, starting with discretized values of incident “latitude” (distance from particle center). A uniform, unidirectional light source was assumed, so that all latitudes experienced the same initial intensity. Only the first through fourth reflections were accounted for, as well as the first through fourth transmissions. A wavelength-specific Sellmeier equation for the index of refraction of soda-lime-borosilicate glass was used, along with Snell’s law and the Fresnel equations, assuming an unpolarized source by averaging S and P polarized reflections and transmissions at each step. Thereby, an expected curve was generated for intensity vs final deflection angle of 632nm HeNe laser light in air, having interacted with a single scattering particle (Fig. 9).

**Figure 8:** Two dimensional ray-tracing geometry depicting incident ray, reflections, and transmissions in a thick spherical shell of glass in air. This particular case shows the ray passing through the central void. In another case, three reflections and two transmissions take place as the ray undergoes total internal reflection (TIR) with the inner surface and then escapes at a final transmission angle. In a third possible case, all light transmitted into the shell undergoes repeated TIR and is bound as a whispering gallery mode. This final case only occurs for light initially incident the highest possible latitude \(R_2\).

**Figure 9:** Theoretical intensities by angle of 632nm light through a thin spherical shell (thickness \(.01R_2\)). This ray-tracing analysis takes separate account of light reflected after one interaction, light transmitted through the central void, and light transmitted after one TIR from the inner surface of the shell. The dotted line is a moving average of the sum of all accounted-for transmissions and reflections.
An empirical curve was then obtained by passing a collimated HeNe beam through a layer of scattering agent averaging one spherical shell in thickness, held in place with a layer of adhesive tape. An Si PIN photodiode in PC mode was swept through deflection angles from 0-80 degrees, where the signal dropped below a noise-level voltage. The experimental and theoretical curves are compared in Figure 10.

![Scattered Intensity by Deflection Angle: Theoretical vs Empirical](image)

**Figure 10:** Comparison of theoretical, empirical intensities by deflection angle. Discrepancies may have been due to slight polarization of laser source, or may have been caused by contact of the scattering particles with an adhesive holding substrate. General agreement, however, suggested that scattering was dominated by the first reflection and was strongly forward-biased. Lack of any observable fine-scale structure within the curve suggested that any diffraction affects could be considered negligible.

The results of this basic experiment showed some discrepancy between theoretical and experimental curves. One source of error may have been a result of the incident laser light being slightly polarized at the source, which did not conform to the unpolarized source assumption used in calculations. Another source of error may have arisen at the interface between the microspheres and the clear adhesive tape. Calculated values assumed a free-floating particle or only a single point of contact at the zero latitude mark, but a contact area between the adhesive layer and scattering particles was visually estimated by microscope in the 10-15 micron diameter range, or approximately 1/5 each bubble diameter. This likely affected results negatively, but two important points were still observed. With a Person’s R correlation factor of 0.887, it did appear that the ray tracing method accounted for the majority of the scattering picture. This suggested that the curve, as predicted, was dominated in intensity by the first reflection in air. It also suggested, in agreement with prediction, that far-field intensity measurements using common photodetection equipment would reveal no appreciable diffraction intensity patterns.

### 2.2. Random Walk Analysis

The core method proposed for the replication of neutron scattering angle probability distributions relies on the employment of multiple scattering events per mean free path. This is because as observed in the open-air experiment, scattering by each particle is expected to be strongly forward-biased and does not match any desired distribution. Therefore, the goal for the model is to predict and employ an averaged angular distribution per mean free path that comes closest to desired material properties as described in section 1.3.2. This method requires an accurate measurement of the probability distribution afforded by a single particle within the chosen substrate, as well as the use of a numerical simulation to predict angular distributions after iterated events.
2.2.1. Empirical Scattering in Resin

The goal of this experiment was to achieve an accurate light intensity vs angle measurement under conditions identical to those found in the final model. In similar fashion to the open-air experiment, a collimated beam of HeNe laser light was passed through a layer of scattering agent and measured at scattering angles from 0° outward (Fig. 11).

In contrast to the open-air measurement, the layer of scattering particles was embedded fully within the same type of resin proposed for the final experiment (commercially-available MAX-CLR-HP 2-part resin). The overall design of the test piece (Fig. 13) employed a semi-circular geometry that eliminated the need to figure transmission angles between resin and air. All angles of incidence and transmission were assumed normal to both the entrance and exit interfaces. Care was taken to ensure that the scattering layer was as close as possible to being one particle thick (Fig. 12). By microscopic inspection, this property was confirmed to an acceptable degree. However, some gaps in coverage were present in the final test piece. Using commonly available image processing software, gaps were estimated to comprise 28.9% of the surface on average. Internal reflection was prevented with the addition of highly absorptive layers on the upper and lower surfaces, as well as the face containing the entrance aperture. These surfaces were prepared by coating the surface with resin and impregnating the layer with black printer toner, which absorbs very efficiently across all pertinent wavelengths. The surfaces were treated again with black enamel after the resin had cured. As before, an SI PIN photodiode was used to measure an output voltage curve (analogous to intensity) at varying deflection angles (Fig. 11). Measurements were taken from 0 to 90 degrees (Fig. 14), where the measured voltage dropped to noise level. It was assumed that the end behavior of the curve after 90° continued to approach zero with a shallow linear slope of $1.5 \cdot 10^{-4} \nu$, as predicted in the discretized tabulation described in section 2.1.

![Figure 11. Apparatus for measuring intensity vs deflection angle after scattering by glass microshells embedded in resin](image)

![Figure 12. Approximate Single-particle layer of scattering agent. Note undesired gaps present. Coverage was estimated with imaging software at 71.1%](image)

![Figure 13. Test Piece for measuring scattered intensity at angles from 0° to 90°. Spherical microshells are embedded in a layer of the same resin that comprises the rest of the sample.](image)
Also depicted in Figure 14 is a corrected version of the curve which features a reduced peak value. This correction was applied to account for the 28.9% lapse in coverage of the scattering layer. A simple reduction factor of 0.7112 was applied to the first three data points which lay within the bright central spot of unscattered light. The final corrected curve was then fitted computationally to an eight-variable rational function with a high adjusted coefficient of multiple determination (Pearson’s R) of \( R = 0.9975 \).

2.2.2. Iterated Angular Probability Distributions
Assuming the curve-fitted function gave an accurate description of scattered intensity at all deflection angles, the function was redefined as a normalized probability function in a Mathematica simulation. For the complete script, see appendix A. In this random-walk simulation, a dataset was generated consisting of 10,000 vectors, each forming an angle \( \theta \) with an initial vector \( \hat{x} \). Angles were randomized in accordance with the defined angular probability distribution. The azimuthal direction of each vector was randomized while preserving \( \theta \). Magnitude was ignored, as it did not affect the iterative process. Figure 15 plots this “first generation” of vectors on a common origin.

After plotting a histogram of resultant angles and verifying conformance to the original probability distribution, the first-generation vector set was used as an input for an iterated algorithm\(^1\). At every step, each of the vectors was subjected again to the curve-fitted distribution to determine its angle with the previous vector. Its orientation was randomly clocked to simulate chance interactions with randomly-placed scattering particles in the optical model. At each of 25 iterations labelled with an index number \( n \), a smooth histogram gave a representation of resultant angles formed with the initial \( \hat{x} \) vector. In this way, it was seen how the angular probability distribution would likely change after \( n \) subsequent interactions.

\(^{1}\) Alternatively, the first generation of vectors could have been replaced by a set of 10,000 initial \( \hat{x} \) vectors. The chosen method allowed for some experimentation in the coding process, and was not intended as the most straightforward approach.
In order to choose a final scattering particle density $N_p$ which is multiplied by the factor $X$ as outlined in section 1.3.2, a target distribution needs to be identified. Equation 13 provides a distribution for any given atomic species, and was solved in another Mathematica script (see Appendix B) to generate the normalized probability curves in Figure 16. In agreement with both Equation 13 and the average-value relation $\langle \cos \theta_{LAB} \rangle = \bar{\mu} = 2/3A$, the distributions move with subsequent values of $A$ from a strong forward bias to more constant probabilities until a near-uniform distribution is reached in the heaviest elements. It is exactly this type of progression that the iterative scattering process is hoped to approximate.

While comparing these angular distributions to those generated in the simulation, we must consider that the curves in Figure 16 were derived through the use of differential cross sections, which described how the probability of interaction varied in relation to resultant azimuthal direction (Eq. 10). For this reason, a perfectly isotropic distribution in this representation would appear as a constant function. In contrast, a simulation that counts angles between any initial vector and a perfectly isotropic array will (somewhat counter-intuitively) reveal a strong peak at the angle of 90°. Figure 17 shows how the simulation approached an isotropic distribution in exactly this manner.

In order to make a fair comparison of these distributions and to settle on a final value of $X$, each resultant vector set was re-characterized in a differential operation which accounted for the rate at which vectors can be found at given polar angles. In rectangular coordinates, the vectors were sorted by angle with respect to $\hat{x}$ into bins of 1° width. Each bin count was then divided by the integrated surface area on the unit sphere corresponding to that particular 1° polar range in spherical coordinates, assuming azimuthal symmetry. This process was repeated for each iterated vector set, as well as for a large sample of highly-randomized vectors (Fig. 18). In this way, the results of the simulation were given in the same differential representation as those in Figure 16.
The final results of the random-walk simulation (Fig. 19) began to show some similarity to target distributions. Because of the limited sample size used, and also most likely due to the initial distribution and the pseudo-random nature of computational vector generation, some unexpected behaviors were observed. Accordingly, some circumspection was applied when interpreting the plots. In particular, the marked uptick at angles nearing 180° was somewhat suspect, and may have occurred as a result of some previously unnoticed end behavior inherent to the fitted curve. However, it was possible to gain some insight from these results with regard to the scattering properties of K15 glass microspheres. Specifically, a consistent peak at the smallest scattering angles seemed to reflect a persistence of forward bias in the system. Such trends are common and well-studied in random walks where the angular distribution afforded by a single particle is highly forward-biased. This type of “persistent random walk”, having a single-step memory (each scattering event depends on the direction of only one preceding step) is commonly characterized in three dimensions by the diffusion coefficient \( D = \frac{\Sigma_{tr}}{3} \), where the transport mean free path \( \Sigma_{tr} \) is defined as \( \Sigma_{tr} = \Sigma_s (1 - \mu) \). The diffusion coefficient is proportional to the mean scattering angle given in a single event. Since calculating the diffusion coefficient requires the density of a particular material and also depends on collision energy, it is not meaningful to generate plots of \( D \) by atomic mass number \( A \). However, a plot can be made of \( \mu \), the average scattering angle cosine. Figure 20 shows this trend, as well as the trend in simulated \( \mu \) at each iteration of the random walk. Note that while both plots utilize the same horizontal-axis values, the mass number \( A \) and the iteration number \( n \) should not be interpreted as having any direct relationship.

**Figure 18.** Histogram plots of angles found in a large-sample (500,000) pseudo-randomly generated vector set with respect to the \( \hat{x} \) vector in \( \mathbb{R}^3 \). Noise arises as a result of less-than-perfect randomization. Plots are given in ordinary histogram count (left) and in the differential representation (right) with respect to the changing area on the unit sphere corresponding to each 1° bin width.

**Figure 19.** Differential scattering angle distribution by sequential iteration. Because bin counts in each 1° range were somewhat sporadic over short intervals, the curves were smoothed by local averaging to obtain a general trend (a much larger sample size would have also aided this purpose).
As seen by the similarities in the trends of figure 20, both the repeated microsphere scattering and the neutron scattering systems smoothly approached isotropy, albeit on different scales. This seemed promising in spite of the visible differences in distributions found in figures 15 & 18. In the process of choosing a final value for $X$, given a particular atomic species and collision energy, most accurate way to compare iterated distributions should be to match as closely as possible the simulated and theoretical values of $\bar{\mu}$. Note that while the iteration values $n$ are only whole numbers, the particle density multiplication factor $X$ need not be. For example, following the red line in Figure 19 seems to imply that the optimal $n$ value to match $\bar{\mu}$ of $^9\text{Be}$ is about 18.5.

2.2. Experimental Verification

Though final decisions on any target materials or specific values of $X$ are left out of the scope of this work, recommendations are hereby made for final testing.

2.2.1. Spatial Neutron Distribution Model

With all system constraints in mind, a possible experimental configuration can be designed which would be capable of modelling a steady-state neutron scattering distribution. Considering ease of manufacture and computational modelling, a sensible first article might consist of a simple rectangular slab of castable resin with a measured amount evenly distributed scattering media embedded within (Fig. 21). An aperture on one end of the slab would serve as a source which would be treated to provide a highly scattering (isotropic) surface. One side of the slab would act as an output which could be scanned via CCD camera. Using a shortwave UV source outside the detection range of the CCD, the measurement surface would be treated with UV reactant fluorophore which would serve to mark intensity at the surface and also to quell internal reflection. All other surfaces would be treated with a highly absorptive material to prevent in-scattering (in the same manner as the test piece shown in figure 13), thus simulating an infinite vacuum boundary.
Dimensions and optical properties for a first-article test should be chosen to emulate a rectangular slab of material with a mean free path in the centimeter range. One such material is \(^9\)Be, a commonly-used neutron reflector. The length of the slab, about 15cm, might conform to the approximate radial thickness of a reflector designed for a recently proposed nuclear-thermal rocket\(^8\), and an initial neutron energy of 2MeV should be chosen in accordance with the average Watt spectrum fission neutron energy. The mean free path at 2MeV for \(^9\)Be is approximately 5cm. Equation 2 shows us how the slowing-down decrement \(\xi\) trends with the atomic mass number \(A\) of a material. While the number of collisions \(n\) needed to reach the thermal energy regime is 18 on average, the greatest energy loss will occur in the first collision. The slowing-down decrement \(\xi\) of \(^9\)Be is about 0.207. From Equation 2, we get \(E' = 0.813E, E'' = 0.661E, E''' = 0.537E\), and so on. Thus after a minimum distance of 15cm travelled, light exiting the model farthest from the source will represent neutrons having undergone at least three thermalization steps and having reached a kinetic energy of around 1.07MeV or less.

As for choosing the correct amount of scattering agent to add to the substrate, the calculation is fairly straightforward. Continuing with the example of \(^9\)Be, and at the incident energy of 2MeV, the published value microscopic scattering cross section \(\sigma_s = 1.657b\). Together with the density of the material, the scattering mean free path comes to \(\Sigma_s = 0.204cm^{-1}\). This is the mean free path that must be used as a starting point for the optical model. Using the average particle size to calculate a cross-sectional area \(a\) for one spherical shell, the particle density \(N_p\) is found (when \(X=1\)) by \(\Sigma_s = 0.204cm^{-1} = N_p a\). With a cross-sectional area of \(a = 2.827 \times 10^{-5}cm^2\), the desired number of scattering particles per cubic centimeter comes to \(N_p = 5,658,000\) particles \(\cdot cm^{-3}\).

Using a published value\(^6\) for the density of bulk K15 microshell powder, the number of particles per gram can be approximated. This involves the employment of the close random packing formula \(\rho = V_{spheres} / V_{cubic vol}\), where \(\rho \approx 0.74\) for tightly-packed spheres. Given that the spheres in this case cannot be assumed closely packed due to their low mass and their dielectric properties, a more reasonable assumption for the ratio \(\rho\) might lie closer to 0.64 (More careful microscopic inspection should be applied to arrive at a best estimate). This would bring the approximate number of particles per cubic centimeter of bulk powder to 5,658,000 particles \(\cdot cm^{-3}\).

This information must then be used to find the ratio of volumes of resin to powder, and finally the masses needed to make a particular volume of mixture. Using the multiplication factor \(X\) found in the simulation, a final concentration of scattering can be mixed uniformly within the castable resin medium. The final test is conducted with the workpiece prepared as shown in Figure 20. The UV light source is applied, and resultant emissions are recorded via CCD camera across the measurement surface. A 3D plot is generated and smoothed for noise by local averaging, and data is checked for final conformity with an MCNP-generated dataset.

2.2.2. Energy Deposition Model

The same general arrangement could also be used to model energy deposition by neutrons (or gamma rays, if desired) within the solid (Fig. 22). In this configuration, fluorophore particles embedded within the bulk of the material energy deposition could be mapped spatially to a significantly accurate degree. Again, all surfaces would be treated with absorptive material, save for the measurement surface which in this model would be chemically etched to reduce internal reflection of source UV rays.
The energy deposition model would not incorporate scattering particles, thus any internal reflection of fluorophore emissions would be absorbed upon incidence with the opposing internal surface and should no longer be detectable. As fluorophore emissions are isotropic in nature, intensity measurements at the surface of the energy deposition model would rely on the spherical symmetry of emitted rays as averaged over some yet-unknown spatial scale (Fig. 23). In the case of a smooth measuring surface, this would hold true out to the critical angle, where point intensity would no longer be convoluted with emissions from fluorophores farther than \( d = \cos(\theta_c) \). A very fine, uniformly etched surface should serve to buffer this convolution limit, as well as to reduce internal reflection of UV source light. A relatively thin slab should be chosen, at least for preliminary measurements, to reduce internal convolution. As with the distribution model, a final array of CCD output voltages would need to be checked for conformity to an MCNP benchmark. Only the intensity pattern of either model with respect to peak magnitude need be examined; overall intensity will be a function of source magnitude and can be ignored until such time as these optical systems are integrated with reactor simulation software.

**Figure 22:** General experimental design for measuring fluorophore emissions within an optical medium. The upper surface transmits local averages of spherically-symmetric emissions from points within the medium.

**Figure 23:** Spherical symmetry of fluorophore emissions results in a local averaging of surface intensity in the neutron energy deposition model, except at incidence angles greater than \( \theta_c \). An etched surface is intended to buffer this convolution limit, as well as to reduce internal reflection of UV source light.
3. Conclusion
Having gone over much of the background material pertaining to lab-reference-frame neutron scattering in solid materials, we have identified a number of similarities with optical ray scattering. Both systems are examples of single-step memory persistent random walks, and their scattering angle probability distributions can be shown in differential representation to approach isotropy with increasing atomic mass number \( A \) in the neutron scattering case, or with sequential scattering iteration \( n \) in the optical ray scattering system. The random walk simulation showed a very smooth evolution in the curve of the average scattering cosine \( \mu \), and though the curve progresses at a slower pace with respect to \( n \) than the neutronic system progresses by \( A \), it should be possible to match a given neutronic distribution by curve matching \( \mu \) in the manner demonstrated in Figure 20. After using this method to find a scattering particle density multiplication factor \( X \), a final test of the optical medium as depicted in Figure 21 should reveal the closest possible representation of a scattered neutron spatial distribution.

There may, however, be sources of error in the optical system that would need to be addressed. Optical resolution will not match the resolution capabilities of an MCNP simulation, but should begin to gain validity at perhaps the millimeter scale where the scattering particles can be treated as points. Another feature of the optical system which will need to be assessed is its need for multiple scattering events per neutron mean free path, as seen in Figure 6. To speculate, this property may either positively or negatively affect the outcome. Since simulated neutron paths will curve more gradually instead of attaining a net deflection in a single event, final intensity distributions across a given plane may suffer. On the other hand, increasing the density of scattering particles may improve the spatial resolution of the system by allowing diffusion to evolve more smoothly.

The scattered neutron distribution model and the energy deposition model are both in preliminary stages of development, and were chosen for their balance of achievable results and ease of production. In theory, it should be possible to imagine much more advanced techniques for managing angular distributions, boundary behavior, and convolution of intensity measurements. There should be no great barrier to prevent test articles being made to the shape of reactor components and placed adjacent to one another to simulate reactivity effects.

Figure 24: Possible arrangement of reactor component analogs in a modular setup for use in educational demonstrations

Figure 24 portrays one possible design of a neutron distribution model having light sources integrated within fuel element analogs which are powered by induction from coils below the stage surface. The upper surfaces of each component are coated with fluorophore, as are the outer boundaries. Each component is designed with internal scattering properties which replicate those of their real-life counterparts, and each piece is moveable so that any arrangement of fuel elements, modulators, control elements, and reflectors can be laid out.
Such a kit could be combined with simulator software and programmed to adjust light sources to mimic reactor kinetics, feedback, or any desired behavior. One drawback is that internal reflection will impact the validity of the surface intensity pattern whenever there is an open boundary condition. This will pose a problem if parts are to be moved by hand and monitored in real time. If all parts are made with a resin having the same index of refraction, internal reflection should be eliminated to a great degree when parts are mated together with smooth, even surfaces. This limitation may or may not prove a bigger problem than the model’s ability to faithfully replicate scattered neutron distributions.

To date, the efficacy of the methods and materials proposed can be considered unproven. Though similar in many respects, the processes of iterated optical scattering and neutronic diffusion have fundamental differences that must be mitigated in order to achieve any meaningful or useful result. It is likely that no optical system will be able to recreate every aspect neutron scattering behavior, particularly with regard to time, energy, or temperature-dependent variables. However, technology does exist to greatly improve upon the methods explored in this work. If these tools were further developed for analysis, education, or outreach, they could mature into popular features of programs in nuclear science and engineering.

4. Acknowledgements

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5. References


APPENDIX A: Random Walk Simulation Code

Random Walk Analysis

Load Saved Vector Sets;
Get[pirgno.ww];
Get[pirhpgno.ww];
Get[tstngno.ww];

n = 25;

initialvector = (1, 0, 0);
set vector = n - 1;

Define Initial Scattering Angles as a Probability Distribution Using Fitted Curve;

\[ \text{Scattering Angles} = \left\{ \begin{array}{ll}
(1 + b \cdot \text{vector} \cdot (1 - 10^a \cdot \text{vector} \cdot \text{vector}) \cdot \text{vector}) & \text{for } \text{vector} > 0 \\
(1 - b \cdot \text{vector} \cdot (1 - 10^a \cdot \text{vector} \cdot \text{vector}) \cdot \text{vector}) & \text{for } \text{vector} < 0
\end{array} \right. \]

Plot[confirm, (0, 0, 180), PlotRange -> Full, Filling -> Axis]

Stat = ProbabilityDistribution[confirm, \{vector, (0, 0, 180), n, (0, 0, 180)}];

Histogram[RandomVariate[Stat, 5000000], 5000;]

Generate Set of Vectors After One Scattering Event;

nvec = n + 1000;
initialvector = (1, 0, 0);

Fireturns

Flatten[
Table[rotationTransform[RandomReal[{0, 2\[Pi]}], (1, 0, 0)]

[\{\text{v}, \text{w}, \text{z}\} /.
rotationTransform[\{\text{v}, \text{w}, \text{z}\} -> \text{initialvector}, \text{v}, \text{w}, \text{z}\} + \text{RandomVariate[Stat, 1]}]",

\{\text{v}, \text{w}, \text{z}\}, \text{Reals}, 1, WorkingPrecision -> 8]\], \{\text{nvec}\}, \{1, 0\}]];

This generates all the vectors according to the distribution, appending them to a list.

(First[Fireturns] +)

Dempthaw[\{pirgno.ww", Fireturns\}];

Graphics3D[Arrow[\{(0, 0, 0), \}\{\text{Fireturns}, \text{PlotRange} -> 1, Axes -> True, AxesLabel -> \{\text{x}, \text{y}, \text{z}\}\}]

Generate Array of Vectors After \(n\) Scattering Events;

n = 25; (total number of consecutive events)

\text{Here} = n - 1; (number of iterations to do after Fireturns)

Fireturns = Reallist[Flatten[
Table[rotationTransform[RandomReal[{0, 2\[Pi]}], \{(\text{initialvector}[1], \text{initialvector}[2], \text{initialvector}[3])\}

[\{\text{v}, \text{w}, \text{z}\}

\{\text{random} \cdot \text{vector} \cdot (1 - 10^a \cdot \text{vector} \cdot \text{vector}) \cdot \text{vector} \cdot \text{vector} - \text{vector} \cdot \text{vector}

\text{random} \cdot \text{vector} \cdot (1 - 10^a \cdot \text{vector} \cdot \text{vector}) \cdot \text{vector} \cdot \text{vector}

\{\text{v}, \text{w}, \text{z}\} + \text{RandomVariate[Stat, 1]}], \{\text{v}, \text{w}, \text{z}\}, \text{Reals}, 1, WorkingPrecision -> 8]\], \{\text{Here}\}, \{1, 0\}]];

(First[Fireturns] +)

Dempthaw[\{pirgno.ww", Fireturns\}]; (These save the datasets to "my documents")

(\{\text{First}\[\{\text{Fireturns}, \text{PlotRange} -> 1, \text{Axes} -> \text{True}, \text{AxesLabel} -> \{\text{x}, \text{y}, \text{z}\}\}\]}

Plot Histograms of Angular Distributions With Respect to "initialvector" after "n" events;

\text{No}\n
Print[\text{No}];
Plot Smooth Histograms of Angular Distributions With Respect to "initial vector" after "n" events;

Create a Highly Randomized Set of Unit Vectors "Isotropic":

Account for Differential Angular Distribution in "Isotropic" to Represent Isotropy as Uniform Function;

Generate Smoothed Plots of Angular Distributions With Respect to "initial vector" after "n" events, Having Represented Isotropy as Uniform Function;
Comparison of theoretical and computational trends in $< \mu >$

\[ A \sim \text{Normal}(\mu, \sigma) \]
\[ \sigma = \frac{\mu}{\sqrt{n}} \]

Theoretical + Normal + \text{Mean} = \text{Average} + \text{Normal distribution from 1 to n} + \text{Mean}

Table:

<table>
<thead>
<tr>
<th>Mean</th>
<th>StdDev</th>
<th>Normalized</th>
<th>Theoretical + Normal + Mean</th>
<th>Average + Normal distribution from 1 to n</th>
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</thead>
<tbody>
<tr>
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<td>0.1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>0.2</td>
<td>0.2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>0.3</td>
<td>0.3</td>
<td>3</td>
<td>3</td>
</tr>
</tbody>
</table>

Graphics: Arrow (0, 0, 1) & (0, 0, 1) & (1, 1, 1) & (1, 1, 1) & (1, 1, 1) & (1, 1, 1) & (1, 1, 1) & (1, 1, 1) & (1, 1, 1) & (1, 1, 1)
APPENDIX B: THEORETICAL SCATTERING ANGLE PROBABILITY DISTRIBUTIONS CODE

\(\theta C = \text{ArcSec} \left( \frac{2A}{-1 + \cos(2\theta L) + \sqrt{2} \cos(\theta L) \sqrt{-1 + 2A^2 + \cos(2\theta L)}} \right)\);

\(\theta E = 1\);

\(p_{0L} = \frac{\theta E}{4\pi} \left( \frac{\frac{1}{\theta L} + \frac{\theta L}{A} + \cos(\theta C) + 1}{\frac{1}{\theta L} + \frac{\theta L}{A} + \cos(\theta C)} \right)\);

\(p_{0L_{\text{max}}} = \frac{\theta E}{4\pi} \left( \frac{\frac{1}{\theta L} + \frac{\theta L}{A} + \cos(\theta C) + 1}{\frac{1}{\theta L} + \frac{\theta L}{A} + \cos(\theta C)} \right)\);

\(\text{Do}\left[\begin{array}{l}
\text{Print} \\
\text{Plot} \left( \frac{\theta E}{4\pi} \left( \frac{\frac{1}{\theta L} + \frac{\theta L}{A} + \cos(\text{ArcSec} \left[ \frac{\theta C}{2\theta L} + \sqrt{2} \cos(\theta L) \sqrt{-1 + 2A^2 + \cos(2\theta L)} \right] + 1) + 1}{\frac{1}{\theta L} + \frac{\theta L}{A} + \cos(\theta C)} \right) \right), (0L, 0, \pi) \right)
\end{array}\right] \);