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Beyond Renewal Approximations: A 1D Point Process Approach to Linear Transport in Stochastic Media

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ABSTRACT

We present a novel approximate model for monoenergetic linear transport in stochastic media that permits correlations between successive free-path lengths of particle collisions. Our model utilizes collision times determined by a 1D point process, chosen such that perfectly forward scattering along a transect precisely matches ensemble-averaged statistics. In contrast, previous renewal-based non-classical transport formulations only guarantee the accuracy of the first collision time and assume subsequent collision times are independently and identically distributed. By accommodating non-renewal collision times, our model can account for step correlations that emerge in most variability models, including cross-section fluctuations driven by Gaussian processes, transformed Gaussian processes, and the majority of discrete mixture models. We compare multiple scattering predictions from our model to new two-dimensional benchmark simulations featuring transformed Gaussian fluctuations, demonstrating enhanced accuracy compared to renewal approximations.

KEYWORDS: Non-Classical, Stochastic, Point Process, Transect, Step Correlations

1. INTRODUCTION

Particle transport in stochastic media presents significant challenges in various domains, including neutron transport, heat transfer, remote sensing, and tissue optics. Even for homogeneous, monoenergetic, time-independent problems, once the total macroscopic cross section $\Sigma_\mathrm{t}(x)$ is subject to randomness, the only exact method for estimating ensemble-averaged observables, given the presence of scattering, is an expensive double-Monte-Carlo simulation that requires averaging classical simulations across numerous system realizations [1]. Developing non-classical equations to directly approximate transport in stochastic media without generating ensemble realizations is, therefore, highly sought after.

One such approach is a *renewal transport process*, whose integral equation is that of random flights [2,3], shown to be equivalent to a *generalized linear Boltzmann equation* (GLBE) [4]. This approach was inspired by the observation that ensemble-averaged extinction in stochastic systems is often non-exponential [5]. By replacing the Poisson process, which produces exponentially-distributed intercollision lengths in classical theory, with a broader *renewal process* [6], this non-exponential behaviour can be directly exhibited in a transport formalism. However, in a system with scattering, the renewal assumption demands that all subsequent free-path lengths are independent, thus disallowing correlations in successive lengths between collisions ("step correlations"). The accuracy of this renewal assumption for modeling general stochastic media is currently not well understood.

In this paper, we introduce a novel model for monoenergetic linear transport in stochastic media that allows arbitrary step correlations, offering insights into when the renewal approximation is appropriate and providing a more general model for when it is not. Our approach utilizes exact collision-time statistics derived from the case of perfectly-forward (singular) scattering, where transport is restricted to unidirectional flow along a medium transect, yielding collision times determined precisely by a 1D point process. By leveraging known results from time series analysis, we can efficiently simulate collisions along transects

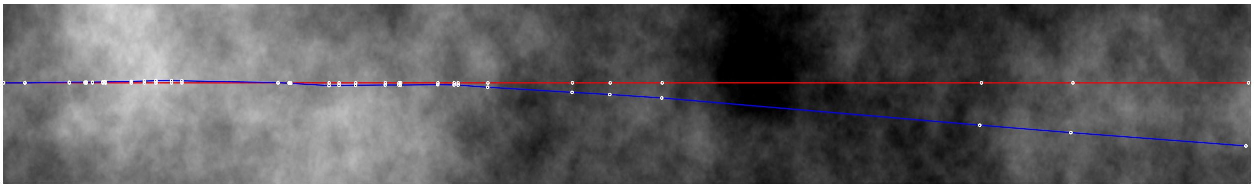

Figure 1: In a realization with fluctuating $\Sigma(x)$ (greyscale), scattering events (white) along a transect (red) are typically correlated (clumpy) and given by a 1D point process. We apply these transect statistics along histories with general scattering (blue).

and rigorously identify which classes of stochastic media are truly renewal. To approximately treat non-forward scattering, we propose applying these transect collision times along a general history, thus creating an efficient autoregressive transport model that directly simulates ensemble-averaged behavior by correlating future collisions with prior times *but not locations* along a history. We demonstrate that our model can outperform a renewal transport process over a wide range benchmarks.

Previous discussions on step correlations in stochastic media have often attributed them to complex correlations emerging when particles scatter backward into prior scenery [7]. While reversal can indeed cause step correlations, we clearly demonstrate that nearly all forms of stochastic media, including those with Gaussian or transformed-Gaussian density fluctuations, exhibit step correlations even in the case of perfectly forward scattering (Figure 1), and therefore step correlations can be expected to arise in nearly all systems, including those with highly forward scattering. To assess the impact of these correlations, we present new benchmark simulations for monoenergetic absorption and scattering in isotropic, stationary two-dimensional (Flatland) stochastic media with transformed-Gaussian density fluctuations. Comparisons between these benchmarks and our new model reveal a reduction in error (relative to a renewal transport process) of up to an order of magnitude.

2. MODEL DEFINITION AND MOTIVATION

In this section, we introduce our novel model, which directly extends the random-flight interpretation of classical linear transport [2,8]. We review essential results from point process literature and explore the role of point processes in determining collision times along a particle history. We then discuss the time-series analysis of collisions along a transect and the relationship to Cox processes, which forms the foundation of our model.

Scope We will limit the scope of the present work to consider only time-independent, monoenergetic linear transport in an isotropic, piecewise-homogeneous medium with deterministic scattering kernel and deterministic single-scattering albedo c. We assume that the total macroscopic cross section $\Sigma_{\text{t}}(x)$ at position x is given by a stationary random field. Extension of our model to time-dependent problems is straightforward. Multi-group, inhomogeneous systems, anisotropic media and stochastic albedo c are not presently supported by our model. Despite these restrictions, we feel that our work unveils important insight regarding the role of step correlations in stochastic systems and the limitations of the GLBE.

2.1. Random Flights and Point Processes

We will determine our model by defining the stochastic process governing a single particle, born at time $t = 0$. Specifically, we will form a generalized random flight by specifying a sequence of random collision times t_i along each history. Our goal is to choose a flight whose expectation directly approximates ensemble-averaged observables in the stochastic system. The collision times t_i constitute a 1D *point process* $N(t)$: a non-negative integer random variable at each time t that gives the number of collisions up to that time [6]. Once $N(t)$ is specified, the transport is completely determined, since the scattering kernel and survival probability c are assumed to be deterministic and independent of t_i. Given $N(t)$, a Monte Carlo estimator for our model is readily derived by sampling collision times t_i from $N(t)$, constructing a history by sampling the scattering kernel at each collision, utilizing implicit capture for absorption, and terminating with roulette or upon escape/boundary interactions.

The Poisson Process of Classical Transport To gain some familiarity with the role of point processes in classical transport, let us recall that in a deterministic homogeneous medium, the collision times along a history are given by a Poisson point process (PPP) with a constant rate $\lambda(t)$ [9]. The PPP is a memoryless point process, where the number of points within a time interval $[t_a, t_b]$ follows a Poisson distribution with a mean of $\int_{t_a}^{t_b} \lambda(t)dt$. Assuming motion occurs at unit speed, the rate of the Poisson process is equal to the total macroscopic cross section $\lambda(t) = \Sigma_{\mathrm{t}}(x(t))$ at the particle's current position $x(t)$. In a homogeneous system, we observe a constant rate $\lambda(t) = \Sigma_{\mathrm{t}}$ and exponential times between collisions. However, in a system with inhomogeneous cross section, such as a realization of a stochastic system, the rate $\Sigma_{\mathrm{t}}(x(t))$ of the point process at time t depends on the current position $x(t)$ (which, in turn, is a function of both prior times *and directions* of the history). Averaging this PPP over the $\Sigma_{\mathrm{t}}(x)$ ensemble becomes intractable.

The complexity of this 3D averaging casts heavy doubt on ever finding an exact random flight approach to general stochastic media. If, however, we constrain the problem to one dimension by either considering only absorption, or forcing scattering to be perfectly forward, exact results are possible. We consider each of these scenarios now, in turn.

Attenuation A number of tractable results are available if we consider only absorption. In this case, transport is restricted to a straight path up to the first collision and the problem is one-dimensional. The *attenuation law* $T(t)$, which is simply the probability of finding no collision in $[0, t)$, is

$$T(t) \equiv \Pr\{N(t) = 0\}. \tag{1}$$

In a deterministic medium, this probability follows from the rate of collisions $\lambda(t) = \Sigma_{\mathrm{t}}(x(t))$ governing the PPP, giving the well-known equation for attenuation

$$T(x) = \exp\left[-\int_0^t \lambda(t')dt'\right] = \exp\left[-\int_0^x \Sigma_{\mathrm{t}}(x')dx'\right]. \tag{2}$$

This equation illustrates a close relationship between the point process and particle transport literatures. In fact, the point process community independently developed the concept of delta (Woodcock) tracking, under the name "thinning algorithm", for sampling events in an inhomogeneous PPP [10,11].

Similarities between these two studies are also found in the case of stochastic rate $\lambda(t)$. For stochastic systems, we denote the *mean attenuation law (from an equilibrium/deterministic origin)* as

$$T_u(x) \equiv \langle T(x) \rangle \tag{3}$$

which is the ensemble average of the deterministic result. Finding $T_u(x)$ requires averaging Equation 2 where Σ_{t} is stochastic, which makes $N(t)$ a doubly-stochastic Poisson process (or *Cox Process*) [12], which was noted by Kostinski [5,13]. The mean attenuation law in Equation 3 is tractable for a number of fluctuation models including Gaussian fluctuations, squared-Gaussian fluctuations and discrete n-ary Markov mixtures.

The 'u' label on $T_u(x)$ refers to an *unconditional* ensemble average over all realizations, and distinguishes the result from an average that is conditioned on starting from $t = 0$ at a scattering center [14]. For brevity, we will consider only deterministic sources, using equilibrium (asynchronous) initialization of the point process $N(t)$ (see [15] for more details). However, synchronous initialization of $N(t)$ is easily adopted for emission from spatially correlated scattering centers, which may be appropriate in neutronics [4].

2.2. Transect Statistics

A Cox process provides a precise and comprehensive representation of transport in a purely absorbing stochastic system, as the absence of scattering reduces the problem to a one-dimensional scenario, allowing for an equivalent 1D point process. Another instance where we can take advantage of this 1D equivalence occurs when the scattering kernel is a singular Dirac delta peak in the forward direction, thus restricting transport to a 1D transect (see, for example, Figure 1). In this case, $N(t)$ is also reduced to a 1D Cox process, accounting for all collisions along the transect instead of just the first one. By eliminating all angular dependence from $N(t)$, we circumvent the intricacies of correlations arising from prior scenery. Although perfectly forward scattering essentially nullifies the scattering collisions, reverting the problem back to one of pure absorption, showcasing these *transect statistics* is still a crucial requirement for any non-classical transport model to be considered accurate. For this reason, we will employ these transect statistics to not only establish a new transport model that embodies them but also to develop new benchmarks for assessing non-classical formalisms.

We now introduce some necessary results from point process literature. Point processes are completely determined by their generating functions. Given a stationary point process, we will denote its *equilibrium probability generating function* as

$$\phi_N(z;t) \equiv \sum_{n=0}^{\infty} z^n \text{Pr}\left\{N(t) = n\right\}, \tag{4}$$

which, for any time t, yields the required probabilities for $N(t)$. The attenuation law along a transect can then be expressed as

$$T_u(t) = \phi_N(0;t), \tag{5}$$

with higher-order probabilities recovered via

$$\text{Pr}\left\{N(t) = n\right\} = \frac{1}{n!}\frac{\partial^n \phi_N(z;t)}{\partial z^n}\bigg|_{z=0}. \tag{6}$$

By giving an exact account of the full point process $N(t)$, the generating function $\phi_N(z;t)$ is a highly useful tool for analyzing the clustering of collisions along a transect in a medium with stochastic cross section (Figure 1). Remarkably, it turns out that determining $\phi_N(z;t)$ is no harder than determining the attenuation law $\phi_N(0;t)$.

For a Cox process, the *optical depth* along a transect is

$$\tau(t) \equiv \int_0^t \Sigma_{\mathrm{t}}(x)dx, \tag{7}$$

which is a random variable. The Cox process is then uniquely determined, given that

$$\text{Pr}\left\{N(t) = k\right\} = \langle e^{-\tau(t)}(\tau(t))^k/k!\rangle, \quad k \geq 0. \tag{8}$$

The probability generating function can then be written [15, p.219]

$$\phi_N(z;t) = \langle \exp[(z-1)\tau(t)]\rangle, \tag{9}$$

which corresponds to the moment generating function of the optical depth at time t, evaluated at $z-1$.

Since $z = 0$ in Equation 9 corresponds to the attenuation law of the Cox process, and because $(z-1)$ simply serves as a constant scaling factor for all optical depths $\tau(t)$ regardless of t, it becomes clear that determining all collision times along the transect is, in fact, no more challenging than determining the attenuation law itself. Said another way: $\phi_N(z;t)$ is just the attenuation law in a system where the random field $\Sigma_{\mathrm{t}}(x)$ is scaled by a constant $(1-z)$.

The Transect Absorption Law We can now define two new analytic benchmarks for measuring approximate non-classical models of transport. Firstly, for an absorbing and scattering system, where each collision scatters perfectly forward with probability c and otherwise absorbs and terminates the random flight, we can solve for the ensemble-averaged attenuation of unit flux $\langle \psi_{\rightarrow}(t) \rangle$ along a transect using the generating function. Given that the attenuation for k collisions occurring along the segment $[0, t]$ is c^k, we have

$$\langle \psi_{\rightarrow}(t) \rangle = \sum_{k=0}^{\infty} \Pr \{N(t) = k\} \, c^k = \phi_N(c; t), \tag{10}$$

which is just the generating function for the point process (Equation 4) evaluated at $z = c$. This result is also equivalent to the attenuation law of a related purely absorbing system where $\Sigma_{\mathrm{t}}(x)$ is scaled by a constant $(1 - c)$ in order to account for the relative probability of real (absorbing) to total (real + null/scattering) collisions. When $c = 0$, the system is purely absorbing and the original attenuation law is recovered, as expected. Likewise, for $c = 1$, the system is lossless and $\langle \psi_{\rightarrow}(t) \rangle = 1$.

Time of the mth collision Another way that we can benchmark non classical models is using the time of the mth collision along the transect. Given the equilibrium generating function $\phi_N(z; t)$ for a stationary point process, the probability density $f_m(t)$ of the time of the mth collision/arrival along a transect (from equilibrium $t = 0$ initialization) is [16, Eq.(25)]

$$f_m(t) = -\frac{\partial}{\partial t} \sum_{j=0}^{m-1} \frac{(-1)^j}{j!} \frac{\partial^j}{\partial z^j} \phi_N(1 - z; t)|_{z=1}. \tag{11}$$

2.3. Non-Renewal Transport

Because transect statistics are a necessary and testable condition for any accurate theory of non-classical transport, we can test the renewal assumption of the GLBE under this lens. This leads immediately to the query: for what class of Σ_{t} fluctuations are the transect statistics renewal, which is to ask: what Cox processes are also renewal processes? This was answered rigorously by Kingman [17]: either Σ_{t} is a two-phase medium with one void phase and exponential chord lengths in the void phase, or Σ_{t} is singular with respect to Lebesque measure. This immediately excludes renewal transport from being a generally accurate model in all but an extremely narrow form of Markov binary mixtures or, alternatively, within media where Σ_{t} is described by some unknown set of fractal variability models. In particular, Gaussian and transformed-Gaussian fluctuations (e.g. Figure 1) are non-renewal and always exhibit clumping of the collision times. It is known that some Gamma and Weibull renewal processes also have a Cox process equivalence, but the exact fractal nature of Σ_{t} that produces them is not known [18].

Approximation by a renewal process To illustrate the non-renewal character of Cox processes with Gaussian fluctuations, we consider the Gauss-Poisson Cox process where $\Sigma_{\mathrm{t}}(x)$ is Gaussian with exponential autocovariance $R(|s-t|) = r^2 e^{-y|s-t|}$, which has a known generating function [6, p.183]. We consider unit mean cross section $\Sigma_{\mathrm{t}}(x)$ and keep r small to make negative cross sections unlikely. In Figure 2, we use the generating function to compare the point counts from equilibrium over various time intervals to those predicted by an equilibrium renewal process. The renewal and Cox processes agree for $n = 0$ (the attenuation law), but all other collision counts differ due to the lack of step correlation in the renewal process. We observed similar inaccuracies of renewal approximations for transformed Gaussian processes (where the Gaussian cross sections are squared or exponentiated to avoid non-negative values), and also when comparing the collision times of the nth collision along a transect, using Equation 11.

2.4. Scattering

Transect statistics have led to several new analytical benchmarks for testing the accuracy of a given non classical theory of transport, but only in the contrived case of purely forward scattering. To form a practical

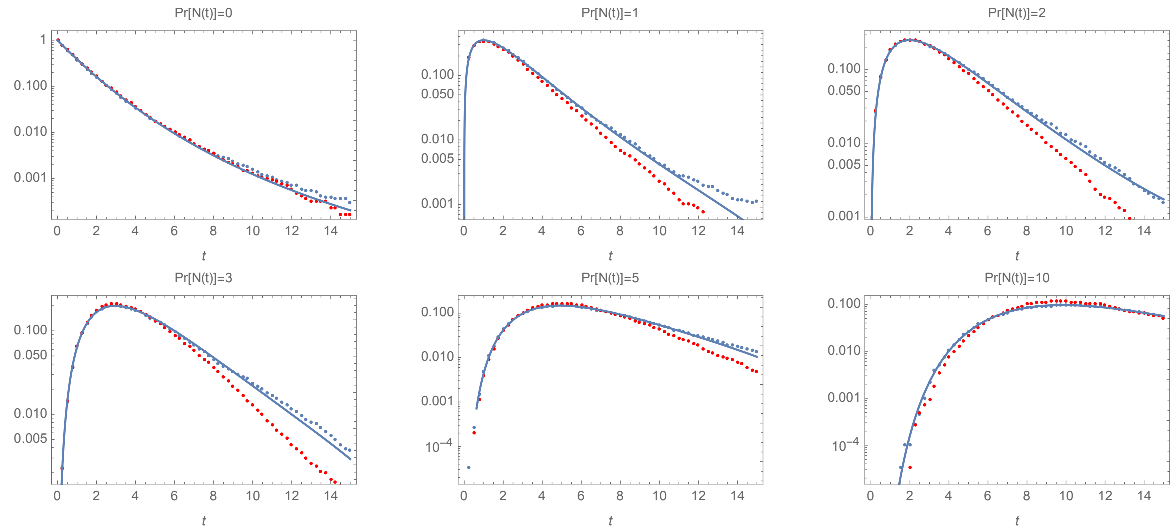

Figure 2: We compare the probabilities for finding n collisions in $[0, t]$ for Gaussian $\Sigma_{\mathbf{t}}(x)$ with exponential correlation $R(|s-t|) = 0.3^2 e^{-0.1|s-t|}$ using double-MC ground truth (blue dots), a renewal process approximation (red dots) and analytic ground truth (continuous). While the attenuation law $n = 0$ matches for the renewal approximation, all other probabilities differ due to the lack of step correlations.

and general model of non-classical transport that exhibits transect statistics, we propose to simply apply them along any history, regardless of the scattering kernel. Intuitively, the clustering of collision times that arises for systems with long-range spatial correlations will be approximately achieved for a system with highly forward scattering (Figure 1). We leave any further justification for the proposed model to numerical benchmark comparisons that we provide in section 3.

We do not presently consider an integral transport equation for our model. This would include a cross section $\Sigma(t_1, \cdots, t_{k-1}; t)$ that is a Janossy density [19] for the point process $N(t)$ up to the current time t subject to the occurrence of $k-1$ prior collisions at times t_i. Such an integral equation could be written down in principle, but it is not immediately clear to us how useful this would be. However, as described above, a Monte Carlo estimator for our model follows directly from the model's definition.

Sampling Transect Collision Times Cox processes can be sampled using a variety of methods [19,20]. For simplicity, in the next section, we sample a single large square tileable auxiliary realization of the stationary random field $\Sigma_t(x)$ using Fourier transforms. This happens once for each piecewise homogeneous element of the system with unique statistics. After this precomputation, traditional Monte Carlo sampling then follows where collision times for each history are determined using delta tracking along a transect in the auxiliary domain. So while a particle in the physical system follows a general history, a virtual particle in the auxiliary domain begins at a random position and direction and follows a straight path in order to determine collision times in the physical system.

Relationship to Prior Work One interesting property of our model is that it includes a number of previous transport formalisms as special cases under a common framework:

- When $N(t)$ is chosen to be a PPP, our model describes classical transport in a deterministic medium.
- When $N(t)$ is a mixed-Poisson process (where Σ is random, but constant in each realization), our model corresponds to an approximation known as the *independent-column approximation* in remote

sensing [21], and is an important benchmark for parametric stochastic media in the limit of infinite correlation lengths.

- When $N(t)$ is a renewal process, $N(t)$ depends only on the previous t_{i-1} collision time, and the resulting integro-differential/integral transport equations are the GLBE/random-flight equations, respectively [2,3,4,14,22,23].
- When $N(t)$ is a Markov-renewal process, $N(t)$ depends only on the previous t_{i-1} collision time and an additional integer state, and corresponds to the chord-length-sampling/Levermore-Pomraning approximations for n-ary Markov mixtures (when we additionally extend the albedos c_j to depend on state j) [24].

3. TESTING THE MODEL

By construction, the accuracy of our model is only ensured in the limited case of purely forward scattering. In this limit, scattering collisions are effectively null events and the transport is equivalent to a purely absorbing one. To test the accuracy of our model for non-forward scattering, we rely on numerical simulations. We constructed a new two-dimensional benchmark for stochastic media with homogeneous mean density, homogeneous deterministic c, and generalized Henyey-Greenstein [25] scattering parametrized by the mean cosine $-1 < g < 1$. The benchmark configuration is illustrated in Figure 3 (left): a deterministic unit monodirectional beam was applied along the normal to the boundary of a source-free disk domain (in two-dimensional Flatland) and the leakage from the vacuum boundary at azimuth ϕ (regardless of outgoing direction) was tallied and averaged over the sampled ensemble of disk realizations. We ran a suite of simulations for Gaussian and transformed-Gaussian Σ_t fluctuations with exponential correlations. In each, we varied the radius R of the disk, the correlation width, as well as c and g.

For each benchmark configuration, we compared the double-MC ground truth result to our new model, and also to a renewal approximation, where the first collision is given exactly and the intercollision lengths were determined in order to form an equilibrium renewal process [14]. For narrow correlation widths, we found close agreement between all three models, and observed deviations as the correlation widths increased relative to the mean free path (see Figure 5). The middle and right plots in Figure 3 illustrate selected examples of the improved accuracy of our model over a renewal approximation for realizations of radius $R = 0.02$ where Σ_t was based on a transformed Ornstein-Uhlenbeck process with radial correlation e^{-r10}, where the Gaussian process was squared to create a non-negative Σ_t field. These examples show substantial improvements over the renewal approximation, both in the highly-peaked $g = 0.9$ case, but, remarkably, also in the more isotropic $g = 0.5$ configuration, where it was less clear that transect statistics should apply. We noted similar behaviour over a wide matrix of configurations, with the renewal approximation being the worst performer overall, and in fact observed our new model consistently outperforming a renewal approximation even in the case of backscattering with $g < 0$ (Figure 4).

We did not perform benchmarks for Markov binary mixtures because our model reduces to the CLS algorithm in such cases and comparisons to a renewal approximation have already been made in 3D [24], where it was also noted that the renewal approximation can significantly underperform relative to a model that includes step correlations (i.e. CLS).

4. CONCLUSION

We have presented a novel non-classical transport model based on transect statistics, which provides a unified framework for various existing transport formalisms. The model has been tested against a range of benchmark configurations, demonstrating its accuracy and robustness even in cases of non-forward scattering. The improvements over the renewal approximation in both highly-peaked and more isotropic configurations highlight the model's potential for practical applications. Our analysis of transect statistics also provides a compelling argument against the use of renewal transport in stochastic systems, casting doubt on the general applicability of the GLBE. Furthermore, the newly established analytical benchmarks for nth collision time and attenuation pave the way for enhanced evaluation and development of future non-classical transport methodologies in multiple fields.

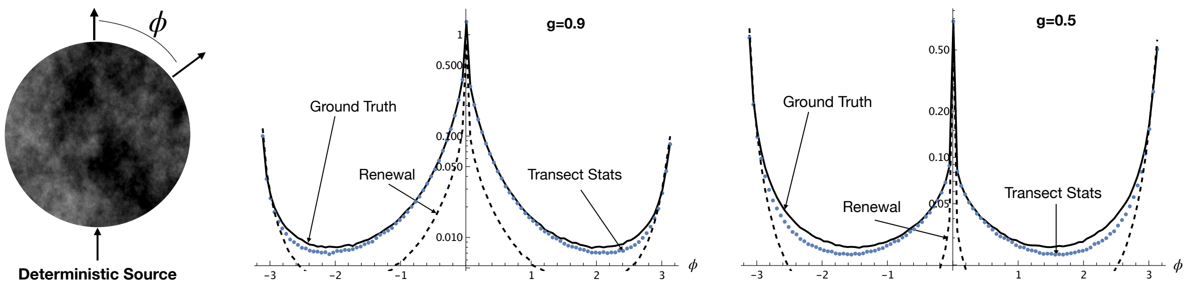

Figure 3: Example benchmark results for the emergent scalar flux when a homogeneous disk domain with stationary fluctuations of $\Sigma_t(x)$ is subject to a monodirectional beam at the boundary. Note how even with a low mean cosine of scattering ($g = 0.5$), our model still significantly outperforms a renewal approximation.

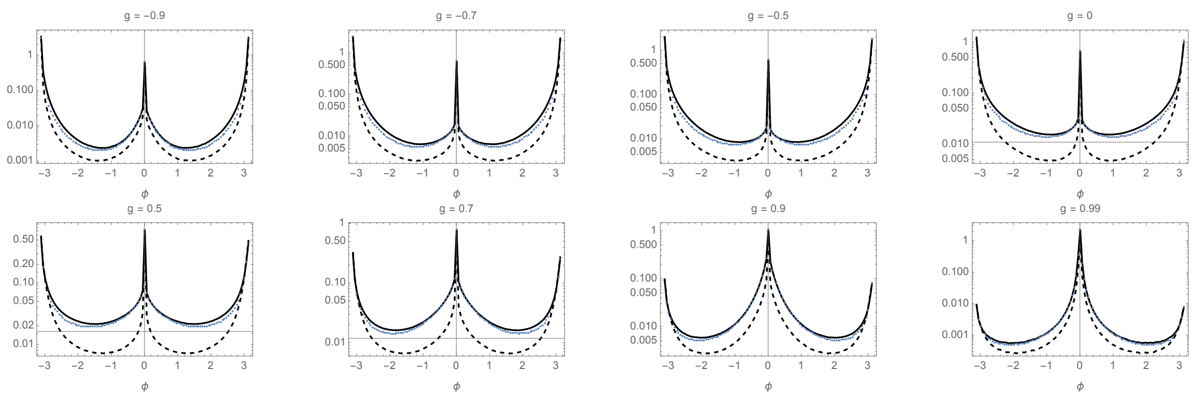

Figure 4: Disk benchmark values comparing ground truth (black) to our model (dots) and to a renewal approximation (dashed) as the mean cosine of scattering g is varied. Note how our model improves upon the renewal approximation even for $g < 0$, which is predominantly back scattering.

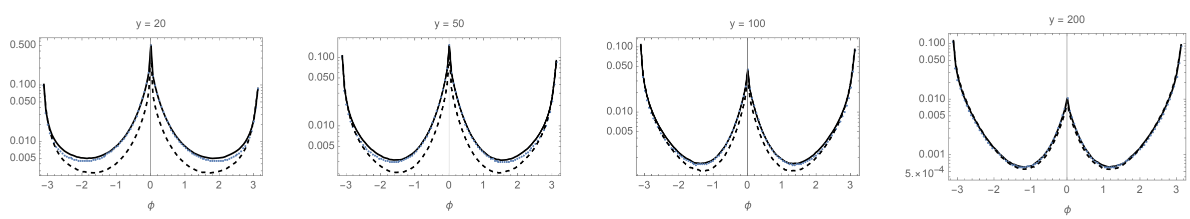

Figure 5: Disk benchmark values comparing ground truth (black) to our model (dots) and to a renewal approximation (dashed) as the correlation parameter y is varied. Note how as y is increased (decreasing the the correlation width of the exponential autocovariance), the variabililty of the fluctuations averages away to a classical medium and all three predictions align.

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