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Nonexponential Radiative Transfer: Reciprocity, Monte Carlo Estimation and Diffusion Approximation

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After more than 125 years of continued utility in many fields, radiative transfer is undergoing a nascent generalization, termed Generalized Radiative Transfer (GRT) [1], to consider light and neutral particle transport in stochastic volumes with spatially correlated scattering centers. Nonexponential random flights have been studied for a long time [2], and stochastic mixtures for several decades [3], but the Boltzmann equation for nonexponential random flights is rather new [4] and requires a number of changes to classical linear transport methodology to apply it in bounded domains. In this talk, we consider, specifically, such changes required for reciprocity, Monte Carlo estimation, and moment-preserving diffusion approximation.

Reciprocity Audic and Frisch [3] proposed the first consistent nonexponential transport formalism for bounded domains, noting the necessity for distinct free-path length statistics $p_c(s)$ between collisions, versus $p_u(s)$ for paths beginning at the boundary (a deterministic location having no correlation to the scatterers). The two "non-Beerian" attenuation laws are $X_c(s) = 1 - \int_0^s p_c(s')ds'$ between collisions and $X_u(s) = 1 - \int_0^s p_u(s')ds'$ from the boundary. Audic and Frisch estimated $p_c(s)$ from Monte Carlo simulation in explicit realizations of the stochastic media. We prove that, for Helmholtz reciprocity to hold in a half space, the two statistics are simply related by $p_u(s) = X_c(s)/\langle s_c \rangle$, where $\langle s_c \rangle$ is the mean free path between collisions. Thus, if the attenuation law $X_u(s)$ for the stochastic media is known from a deterministic (uncorrelated) origin, such as the Levermore-Pomraning law for a Markovian binary mixture, then the intercollision free-path distribution is simply

$$p_c(s) = \langle s_c \rangle \frac{\partial^2}{\partial s^2} X_u(s), \tag{1}$$

which agrees with known relationships between the Lineal path function and chord lengths in heterogeneous materials and stereography and is consistent with the only formulation of nonexponential transport that exhibits Cauchy's formulas for path length invariance [6]. We show that Monte Carlo simulation in negatively correlated media supports this formulation, where the difference in statistics is strongly evident (Figure 1).

Larsen and Vasques [4] illuminated the linear transport approach to nonexponential random flights by extending the macroscopic cross section between collisions to remember the distance s since the previous collision via

$$\Sigma_{tc}(s) = p_c(s)/X_c(s) \tag{2}$$

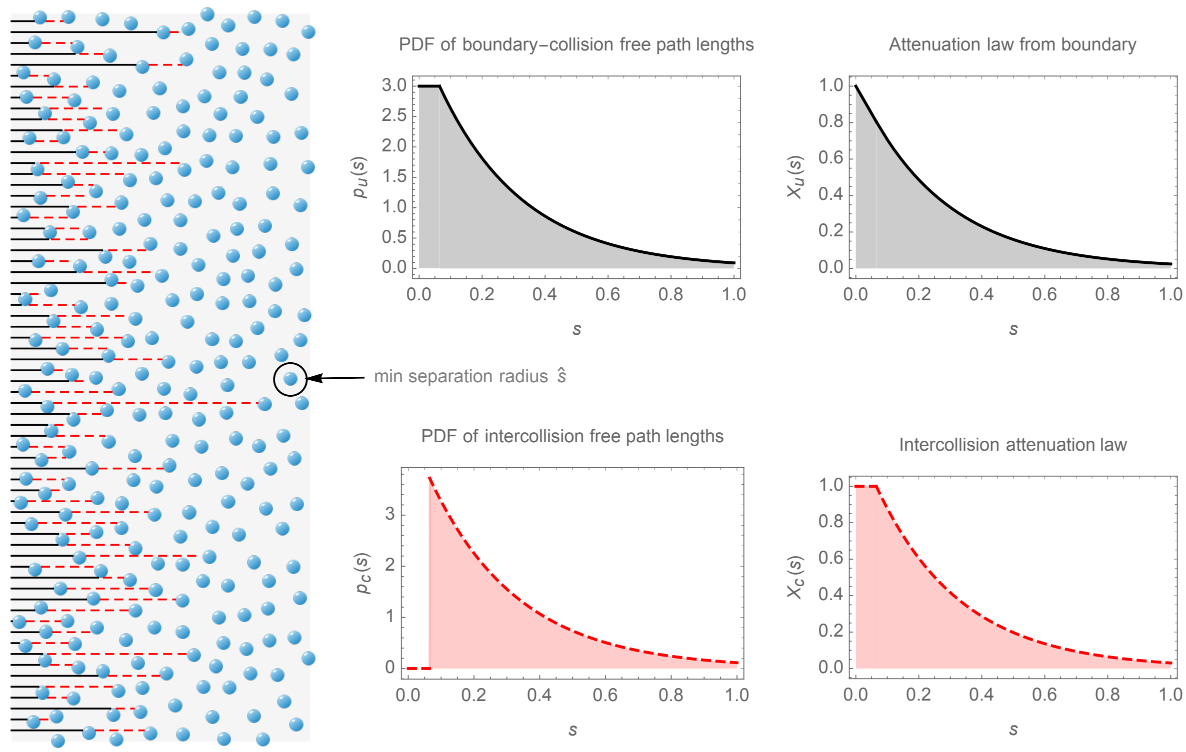

Figure 1. When scatterers in a random medium are spatially correlated, the free-path length statistics between collisions are necessarily distinct from those for paths beginning at a boundary interface. Here we illustrate the case of negatively-correlated convex scatterers separated by a minimum distance $\hat{s} = 0.065$. For paths beginning at the left boundary of a unit thickness slab (solid-black) collisions can occur arbitrarily close to the boundary and the related path length PDF $p_u(s)$ and attenuation law $X_u(s)$ reflect this. Continuing in the same direction from the first collision to the second collision (red-dashed), we find path lengths with a minimum length $\hat{s}$. The intercollision free-path distribution $p_c(s)$ is therefore identically zero for $s < \hat{s}$ due to the scatterers separation, and the attenuation law between collisions $X_c(s)$ is 1 for this initial distance.

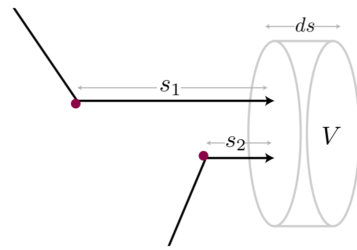

Figure 2. When the scatterers in a homogeneous random medium are spatially correlated, the probability of a collision is track-length dependent. The macroscopic cross section $\Sigma_{tc}(s)$ depends on s, the distance since previous collision, and the probability of collision when traversing a path of incremental distance ds is $\Sigma_{tc}(s)ds$. The collision rate in V is estimated by the traditional collision estimator, scoring the particle weight W for each collision in the region. However, a track-length estimator for the collision rate in V must score $W \int_s^{s+ds} \Sigma_{tc}(s')ds'$ due to the track-length dependence on collision probability. Conversely, for estimating the flux integral in V, the traditional track length estimator, scoring W-weighted track-lengths in V, maintains its familiar form, but the collision estimator must be modified to score $W/\Sigma_{tc}(s)$. If both flux integral and collision rate are desired in V, two distinct tallies must be kept.

and we extend their approach to bounded domains with an equilibrium imbedding of their generalized Boltzmann equation via a distinct cross section for uncorrelated-origins,

$$\Sigma_{tu}(s) = p_u(s)/X_u(s). \tag{3}$$

The distinction between a correlated source, that emits from the spatially correlated microstructure directly, such as in a reactor or thermal emission in a cloud, and an uncorrelated source, such as one entering at a medium boundary, is also required, and explains the two distinct solutions to the Milne problem for binary mixtures noted by Pomraning. It also leads to two families of Green's functions and related diffusion approximations.

Monte Carlo Estimators In GRT, collision rate density and radiance have a nonlocal relationship due to the semi-Markov nature of the random flight, and are no longer interconvertible with a trivial multiplication by Σ_t, requiring distinct estimators and tallies for either physical quantity. The required alterations are summarized in Figure 2. The collision estimator is incapable of estimating fluxes in some cases and we show how fictitious scattering can circumvent this limitation. We derive new exact Green's functions for Gamma-random flights in infinite 3D settings to validate these estimators. We also describe another estimator that can estimate collision rates in a track-length fashion without requiring integrations of the cross-section along each path.

Diffusion Approximation We derive new moment-preserving diffusion approximations for either scalar collision rate or fluence quantities in both the correlated and uncorrelated emission settings in arbitrary dimension. We find in all cases the diffusion coefficients reduce to algebraic expressions involving moments of $p_c(s)$, up to order 4, which we denote,

$$\langle s_c^m \rangle = \int_0^\infty p_c(s) s^m ds. \tag{4}$$

We also derive the modified diffusion approximation method of Grosjean that removes the direct or uncollided portion of the distribution and describes the remaining portion with a diffusion term such that low order moments are preserved. For the collision rate about a correlated source, for general anisotropic scattering with mean cosine g in dimension d, we find the diffusion coefficient

$$D_{C_c} = \frac{\langle s_c^2 \rangle}{2d} \left(1 + cg \frac{2\langle s_c \rangle^2}{\langle s_c^2 \rangle (1-cg)} \right). \tag{5}$$

Grosjean's approximation for the collision rate density C_c is,

$$C_c(r) \approx \frac{p_c(r)}{\Omega_d(r)} + \frac{c}{1-c} m_d \left(\sqrt{\frac{(2-c)\langle s_c^2 \rangle (1-cg) + 2g\langle s_c \rangle^2}{2(1-c)d(1-cg)}}, r \right). \tag{6}$$

where $\Omega_d(r)$ is the surface area of a sphere of radius r in $\mathbb{R}^d$.

For the fluence about a point source with a deterministic origin and isotropic scattering, we find the generalized diffusion coefficient

$$D_{\phi_u} = \frac{\langle s_c \rangle \left(4c\langle s_c \rangle (3c\langle s_c \rangle \langle s_c^2 \rangle - 2c\langle s_c^3 \rangle + 2\langle s_c^3 \rangle) + (1-c)^2 \langle s_c^4 \rangle \right)}{6d \left(2c\langle s_c \rangle^2 - c\langle s_c^2 \rangle + \langle s_c^2 \rangle \right)^2} \tag{7}$$

which, with classical exponential transport, reduces to the well-known

$$D_{\phi_c} = D_{\phi_u} = \frac{(1-c)^2}{\Sigma_t \, d} + \frac{(2-c)c}{\Sigma_t \, d} = \frac{1}{\Sigma_t \, d} \tag{8}$$

with the portion $(1-c)^2/(\Sigma_t \, d)$ arising from the uncollided flux and $(2-c)c/(\Sigma_t \, d)$ from the collided portion.

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