Diffusion approximations for nonclassical Boltzmann transport in arbitrary dimension

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Abstract

In a recent work we derived new diffusion approximations for the collision density and energy density about an isotropic point source in an infinite isotropically-scattering medium in arbitrary-dimensional space with general free-path distribution. In this brief followup we prove several conjectures from our previous paper, show new results for the energy density about the point source, and provide more general derivations that avoid the necessity for any Fourier transforms.

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1 Intro

1.1 New Diffusion Point Source Green's functions

This work is concerned with the distributions of collisions and the density of particles or energy in flight around an isotropic point source in an infinite scattering medium. Specifically, this tech brief presents new compact analytic solutions to two distinct forms of diffusion-based approximations for the infinite-medium point-source Green's function. These new general forms extend previous classical methods to support a nascent form of non-classical linear transport theory where free paths are drawn from an arbitrary distribution, with classical transport theory included as the special case that the free-path distribution is exponential.

This work briefly follows up on a recent paper [d'Eon 2014b], providing more general results that are obtained directly from simple integrals of the free-path distribution, avoiding the machinery of Fourier transforms used previously.

1.2 Related work

This work presents new compact generalizations of the classical diffusion point-source fluence Green's function for the infinite medium,

$$\phi(r) = \frac{1}{4\pi D}\frac{e^{-\sqrt{\Sigma_a/D}\,r}}{r}, \tag{1}$$

which is the core component of many practical analytic BSSRDFs in graphics [Farrell et al. 1992; Jensen et al. 2001; Brinkworth 1964; Donner and Jensen 2005; Donner and Jensen 2007; D'Eon and Irving 2011; Habel et al. 2013; d'Eon 2014a]. The generalizations of this distribution that we present below may lead to useful extensions of the above approaches to support generalized media where the assumptions of classical transport do not apply [Moon et al. 2007; Larsen and Vasques 2011; Meng et al. 2015], in particular, where the free path distribution is not exponential.

We consider the collision density separately from the fluence. We previously noted [d'Eon 2014b] that, in contrast to alternative derivations of diffusion approximations for nonclassical Boltzmann transport [Larsen and Vasques 2011; Frank et al. 2015], a moment-preserving approach yields differing diffusion lengths and forms for the density of collisions around a point source versus the scalar flux or fluence of particles *in flight* about the point source. We further explore this difference here.

2 Setup

We consider multiple scattering distributions about an isotropic point source in a homogeneous infinite medium. We leave the dimension of the medium, d, a general parameter. We require the surface area of the unit sphere in d dimensions

$$\Omega_d(r) = \frac{d\pi^{d/2}r^{d-1}}{\Gamma\left(\frac{d}{2}+1\right)}. \tag{2}$$

2.1 Absorption

Our results apply to transport with classical absorption (capture) with single-scattering albedo $0 < c < 1$.

2.2 Free-path distributions

The distribution of free paths between scattering and absorption events is sampled from the free-path distribution $p(s)$, which is a normalized distribution on $s \in [0,\infty]$,

$$\int_0^\infty p(s)ds = 1. \tag{3}$$

This work additionally requires that the free-path distribution has a finite *mean free path*,

$$\langle s\rangle = \int_0^\infty sp(s)ds \tag{4}$$

and finite *mean square free path*

$$\langle s^2\rangle = \int_0^\infty s^2 p(s)ds. \tag{5}$$

Classical transport theory is included in the special case that the free path distribution is exponential,

$$p(s) = \Sigma_t e^{-\Sigma_t s}. \tag{6}$$

2.3 Diffusion modes

The radial diffusion mode about a point source in an infinite medium of dimension d is

$$m_d(\nu,r) = (2\pi)^{-d/2} r^{1-\frac{d}{2}} \nu^{-\frac{d}{2}-1} K_{\frac{d-2}{2}}\left(\frac{r}{\nu}\right) \tag{7}$$

where $K_n(x)$ is the modified Bessel function of the second kind.

The diffusion mode for the one dimension rod ($d = 1$) is

$$m_1(\nu, r) = \frac{e^{-\frac{r}{\nu}}}{2\nu}, \tag{8}$$

for flatland ($d = 2$) is

$$m_2(\nu, r) = \frac{K_0\left(\frac{r}{\nu}\right)}{2\pi\nu^2}, \tag{9}$$

and for three dimensions is

$$m_3(\nu, r) = \frac{e^{-\frac{r}{\nu}}}{4\pi r\nu^2}. \tag{10}$$

3 Collision Density

In this section we present approximations for the probability density $C_{\text{pt}}(r)$ of particles *entering* collisions at a distance r from an isotropic point source in an infinite isotropically-scattering medium. Our approach is to directly seek a form based on diffusion modes with the requirement that the exact number of collisions and mean square distance of collisions from the source are preserved. Thus, the approximations and the exact solution have identical zeroth and second radial moments,

$$C_0 = \int_0^\infty \Omega_d(r) C_{\text{pt}}(r) dr,$$
$$C_2 = \int_0^\infty \Omega_d(r) C_{\text{pt}}(r) r^2 dr.$$

3.1 Summary

3.1.1 Exact Collision density moments

The first two even moments for the density, $C_{\text{pt}}(r|n)$, of particles entering their nth collisions are

$$\int_0^\infty \Omega_d(r) C_{\text{pt}}(r|n) dr = c^{n-1} \tag{11}$$

and

$$\int_0^\infty r^2 \Omega_d(r) C_{\text{pt}}(r|n) dr = \langle s^2 \rangle n c^{n-1}. \tag{12}$$

The first two even moments for the total collision density $C_{\text{pt}}(r)$ are

$$\int_0^\infty \Omega_d(r) C_{\text{pt}}(r) dr = \frac{1}{1-c} \tag{13}$$

and

$$\int_0^\infty r^2 \Omega_d(r) C_{\text{pt}}(r) dr = \frac{\langle s^2 \rangle}{(1-c)^2}. \tag{14}$$

3.1.2 Classical Diffusion Approximation

The classical diffusion length ν for the collision density is given by

$$\nu = \sqrt{\frac{\langle s^2 \rangle}{2d(1-c)}} \tag{15}$$

yielding the classical diffusion approximation for the collision density,

$$C_{\text{pt}}(r) \approx \frac{1}{1-c} m_d(\nu, r). \tag{16}$$

3.1.3 Grosjean-form Diffusion Approximation

The Grosjean-form diffusion length ν_G for the collision density is given by

$$\nu_G = \sqrt{\frac{\langle s^2 \rangle (2-c)}{2d(1-c)}} = \nu\sqrt{2-c} \tag{17}$$

yielding the Grosjean-form diffusion approximation for the collision density,

$$C_{\text{pt}}(r) \approx \frac{p(r)}{\Omega_d(r)} + \frac{c}{1-c} m_d(\nu_G, r). \tag{18}$$

4 Scalar Flux / Fluence

To determine the density of particles in flight at some radius r from the point source we require the *source extinction function*, related to the free-path distribution by

$$E(s) = 1 - \int_0^s p(x) dx. \tag{19}$$

It is important to recall that, in the case of general media, $E(s)$ only applies to extinction of particles leaving a collision or birth, and does not apply generally to any particle in flight at any location. The last quantity we require to determine diffusion forms is the second spatial moment of $E(s)$,

$$E_2 = \int_0^\infty E(s) s^2 ds. \tag{20}$$

Similar to our approach for the collision densities, we arrive at a energy-conserving approach requiring that the first two event moments of the diffusion approximations match the moments of the exact fluence distribution,

$$\phi_0 = \int_0^\infty \Omega_d(r) \phi(r) dr,$$
$$\phi_2 = \int_0^\infty \Omega_d(r) \phi(r) r^2 dr.$$

Our solutions thus preserve the total energy in flight about the point source as well as the mean-square distance from the source and produce diffusion lengths that are not proportional to the collision diffusion lengths.

4.1 Summary

4.1.1 Exact Fluence moments

The first two even moments for the nth-scattered fluence $\phi(r|n)$ are

$$\int_0^\infty \Omega_d(r) \phi(r|n) dr = c^n \langle s \rangle \tag{21}$$

and

$$\int_0^\infty r^2 \Omega_d(r) \phi(r|n) dr = (E_2 + \langle s \rangle \langle s^2 \rangle n) c^n \tag{22}$$

The first two even moments for the total fluence $\phi(r)$ are

$$\int_0^\infty \Omega_d(r) \phi(r) dr = \frac{\langle s \rangle}{1-c} \tag{23}$$

and

$$\int_0^\infty r^2 \Omega_d(r) \phi(r) dr = \frac{(1-c)E_2 + \langle s \rangle \langle s^2 \rangle c}{(1-c)^2}. \tag{24}$$

4.1.2 Classical Diffusion Approximation

The classical diffusion length ν_ϕ for the fluence is given by

$$\nu_\phi = \sqrt{\frac{E_2(1-c) + \langle s \rangle \langle s^2 \rangle c}{2d\langle s \rangle (1-c)}} \tag{25}$$

yielding the classical diffusion approximation for the fluence,

$$\phi(r) \approx \frac{\langle s \rangle}{1-c} m_d(\nu_\phi, r). \tag{26}$$

4.1.3 Grosjean-form Diffusion Approximation

The Grosjean-form diffusion length $\nu_{G\phi}$ for the fluence is given by

$$\nu_{G\phi} = \sqrt{\frac{E_2(1-c) + \langle s\rangle\langle s^2\rangle}{2d\langle s\rangle(1-c)}} = \nu_\phi\sqrt{2-c} \quad (27)$$

yielding the Grosjean-form diffusion approximation for the fluence,

$$\phi(r) \approx \frac{E(r)}{\Omega_d(r)} + \frac{\langle s\rangle c}{1-c} m_d(\nu_{G\phi}, r). \quad (28)$$

4.2 Numerical Comparison

In Figure 1 we compare the above diffusion approximations for Gaussian random flights in 3D ($d = 3$) with free-path distribution

$$p(s) = \frac{2e^{-\frac{s^2}{\pi}}}{\pi}. \quad (29)$$

Collision density $C_{\rm pt}(r)$ and fluence $\phi(r)$ are compared to Monte Carlo simulations in the same plots. The mean-free path of the random flight is $\langle s\rangle = 1$. The distributions and their Grosjean-form approximations are significantly different for collision density vs fluence. In both cases, we see the Grosjean-form approximation performing well near the source and outperforming the classical diffusion approximation in the highly-absorbing scenario (single scattering albedo $c = 0.3$).

5 Proofs

In the next revision of this tech report, coming soon, we will provide the proof of these results, which follow directly from the Fourier-transformed quantities and their derivatives [Zoia et al. 2011].

6 Future Work

6.1 Generalized Dipole and Multipole BSSRDFs

A generalized diffusion dipole model [Farrell et al. 1992; Jensen et al. 2001] could in theory be derived for non-classical non-exponential random media using Equation 26 (and its depth gradient) for the fluence poles to generalize the flux balance and exitance distributions at the boundary of a semi-infinite medium. Equation 28 would extend this model in the "better" dipole fashion [d'Eon 2012]. Analagous extensions for the multipole BSSRDF [Donner and Jensen 2005] are possible.

Extended-source (photon beam) models [Farrell et al. 1992; Donner and Jensen 2007; D'Eon and Irving 2011; Habel et al. 2013] would likewise generalize using the general free-path distribution $p(s)$ to distribute fluence poles and their negative mirrors within the medium at each location of first collision. A dual beam method [d'Eon 2014a] would, however, use a collision-density approximation (Equation 18) interior to the medium at the poles (instead of fluence), with a detector beam employing the source-extinction function (Equation 19) to attenuate particles leaving collisions and escaping uncollided after their last bounce.

This difference speaks to one important and subtle aspect of generalized transport. With non-exponential transport, the fluence is no longer proportional to the density of collisions times the scattering coefficient Σ_t because $\Sigma_t(s)$ now depends on the free path variable s. Thus, knowing the radiance or fluence at some point in the medium is insufficient information for determining the nearby radiance and evolution of the transport—a complete breakdown of radiance $L(s)$ is required [Larsen and Vasques 2011]. Simple extinction calculations are no longer possible—the source-extinction function only applies to energy leaving a collision or birth. In forward or adjoint random walks estimators of generalized transport, Equation 19 can be used for next-event estimation from sampled collisions only. Care must be taken that all reduced-intensity calculations and track-length (photon beam) estimators use the source extinction function (Equation 19) to *integrate only collision densities and not fluence*. For complete accuracy, the full free-path s breakdown of the radiance and fluence must be preserved for all transport acceleration techniques (this was not the case in the sphere-acceleration method of [Moon et al. 2007] where s was reset to 0 after leaving each acceleration sphere).

6.2 Open Problems

The above generalizations will require answers to two open problems.

6.2.1 Free-path initialization upon entering the medium

As Frank et al. [2015] point out, correct initialization of the free path parameter s upon entering a semi-finite or finite medium remains an open question. Initialization to 0 might be tempting, but it seems more likely that some probability weighted initialization of s will prove most accurate, which may complicate the resulting BSSRDFs significantly.

6.2.2 Generalized diffusion boundary conditions

Finally, classical diffusion boundary conditions are typically based on solution to the Milne problem [Aronson 1995], which, to our knowledge, has no published generalization for general free path transport.

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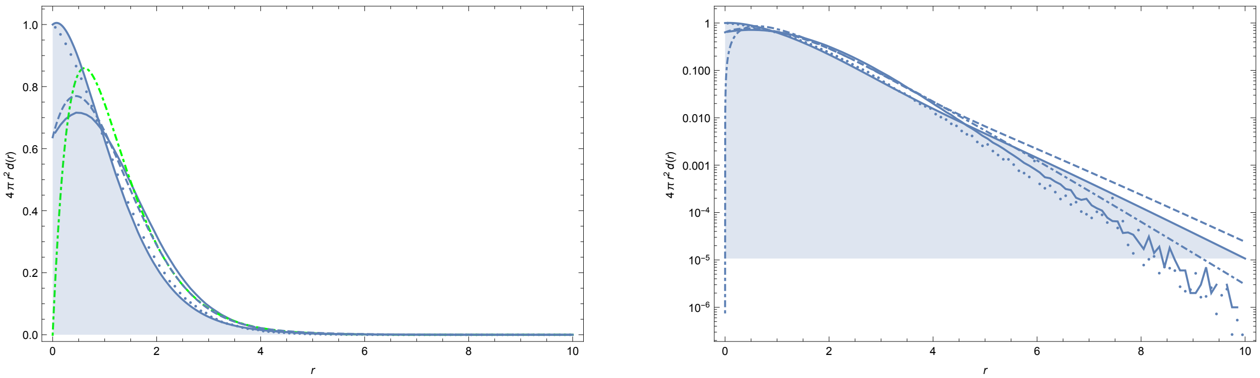

Figure 1: *Uniform (left) and log (right) plots of a variety of Ω-weighted distributions $d(r)$ for Gaussian random flights with $c = 0.3$ in 3D. The fluence $d(r) = \phi(r)$ is compared in filled (Grosjean) and circles (Monte Carlo). The collision density $d(r) = C_{pt}(r)$ is compared in green-dot-dashed (classical diffusion), dashed (Grosjean) and non-filled-continuous (MC).*

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